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BENCHMARK-76: MODEL COMPUTATIONS FOR DISTURBED ATMOSPHERIC COND--ETC(U)  
MAR 78 J M HEIMERL, F E NILES

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BENCHMARK-76: MODEL COMPUTATIONS FOR  
DISTURBED ATMOSPHERIC CONDITIONS.

II. RESULTS FOR THE STRATOSPHERE AND MESOSPHERE

J. M. Heimerl  
F. E. Niles

March 1978



US ARMY ARMAMENT RESEARCH AND DEVELOPMENT COMMAND  
BALLISTIC RESEARCH LABORATORY  
ABERDEEN PROVING GROUND, MARYLAND

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## INTRODUCTION

We have employed BENCHMARK-76, a version of the AIRCHEM<sup>1</sup> code with a 64 species set and a nominal 496 reaction set to obtain species densities as a function of time and altitude for the following disturbed conditions. The prompt ionization,  $N_0 = 10^{11} \text{ cm}^{-3}$  and the delayed ionization is given by

$$Q(t) = Q_0 (1 + t)^{-1.2}, \quad (1)$$

where  $t$  is the time in seconds and  $Q_0 = 10^8 \text{ ion-pairs/cm}^3\text{-s}$ . The relative distribution of the species:  $N_2^+$ ,  $O_2^+$ ,  $N^+$ ,  $O^+$ ,  $N(^4S)$ ,  $N(^2D)$ ,  $O(^3P)$ ,  $O(^1D)$ ,  $O_2(a^1\Delta)$  and  $O_2(b^1\Sigma)$  produced by ionization under disturbed conditions is taken to be: 0.64, 0.16, 0.14, 0.06, 0.45, 0.61, 1.28, 0.10, 0.24 and 0.05 particles per ion pair, respectively. This distribution closely follows that of Gilmore,<sup>2,3</sup> except that  $[O_2(^1\Delta)]$  is taken as 0.24 and  $[O]$  is 1.28. Cases for daytime and nighttime conditions are reported; the calculations correspond to about a three hour interval centered around noon and midnight. Appropriate neutral densities have been outlined elsewhere.<sup>4</sup> The program coding and fixed-input parameters have been previously discussed.<sup>5</sup> Results were obtained from the BENCHMARK-76 program for the altitude region 10-80 km inclusive for daytime conditions and 30-80 km for nighttime.

It is the purpose of this report to: (1) display selected computed results as a function of time and/or altitude, (2) show the results of comparison and sensitivity studies of a very limited nature, (3) report the temporal and altitude variations of the computed equivalent rate coefficients (ERC's), and (4) indicate the type of detailed analysis available from the BENCHMARK-76 output. (A copy of these BENCHMARK-76 results may be obtained by writing the authors.)

<sup>1</sup>E. L. Lortie, M. D. Kregel and F. E. Niles, "AIRCHEM: A Computational Technique for Modeling the Chemistry of the Atmosphere," BRL Report No. 1913, August, 1976. (AD# A030157)

<sup>2</sup>F. Gilmore as quoted by B. F. Myers and M. R. Schoonover, "Electron Energy Degradation in the Atmosphere: Consequent Species and Energy Densities, Electron Flux, and Radiation Spectra," DNA 3513T, 3 Jan 75, Table 6.

<sup>3</sup>J. M. Heimerl and F. E. Niles, "BENCHMARK-76: Model Computations for Disturbed Atmospheric Conditions I. Input Parameters," BRL Report No. 2022, October 1977. (AD #A050355)

<sup>4</sup>F. E. Niles and J. M. Heimerl, "Selected Neutral Species Profiles 0-100 km," BRL Memo Report No. 2767, July 1977. (AD# A042620)

## RESULTS

### A. Selected Densities

The electron density computed as a function of time is shown for each decade of altitude for day and night conditions in Figures 1 and 2, respectively.  $Q$ , the electron production as a function of time is shown at the uppermost section of each figure. The smooth curves were drawn between computed values at 1, 2, 4 and 7 units of each decade in time.

Except at 80 km during the night and above 60 km during the day it appears that by  $10^4$  seconds the electron decay follows the production function decay. Three-body attachment is the dominant electron depopulating process at late times (except at 70 km and 80 km) and  $Q$  is the dominant production mechanism (except for late times at 80 km during the day). The reason for this peculiarity is discussed below (Section E) as an example of the detailed analysis available from the BENCHMARK-76 output.

Some of the curves cease abruptly in these (and other) figures because computations are automatically halted whenever the electron density falls below  $10\text{ cm}^{-3}$ , the assumed quiescent background electron density.

Figures 3 and 4 show the sum of the negative ions (exclusive of electrons) computed as a function of time. Conditions correspond to those in Figures 1 and 2, respectively. Figures 5 and 6 show the corresponding plots for the sum of the positive ions. This sum is insensitive to day/night conditions. To avoid crowding, odd decades of altitude have been plotted in Figure 5 and even decades in Figure 6.

### B. Comparison

Figures 7 and 8 show the electron density computed as a function of time at 60 km altitude for both the BENCHMARK-76 results (BRL-76) and the DCHEM results of Scheibe<sup>5</sup> for daytime and nighttime, respectively. Figures 9 and 10 show similar comparisons for the total positive and negative ions under daytime and nighttime conditions, respectively. The agreement is very good to excellent. These two codes employ different integration schemes and different overall chemistry.<sup>6</sup> However, a detailed examination of the controlling chemistry at 60 km might show strong similarities. Such an examination is beyond the scope of the present report. Comparisons made for other values of  $Q_0$  and  $N_0$  show basic agreement of results of these two codes. We take these comparisons to indicate that the agreement is real rather than fortuitous.

<sup>5</sup>W. S. Knapp, "A Simplified D-Region Chemistry Model for Nuclear Environments," DNA-2850T, April 72; also M. Scheibe, Mission Research Corporation, private communication, 1976.

<sup>6</sup>For example, The BENCHMARK-76 reaction set includes neutral odd-hydrogen reactions, while Scheibe's set does not.

<sup>7</sup>J. M. Heimerl and F. E. Niles, "BENCHMARK-76: Model Computations for Disturbed Atmospheric Conditions III. Results for Selected Excitation Parameters at 60 km," BRL Technical Report ARBRL-TR-02051, March 1978.



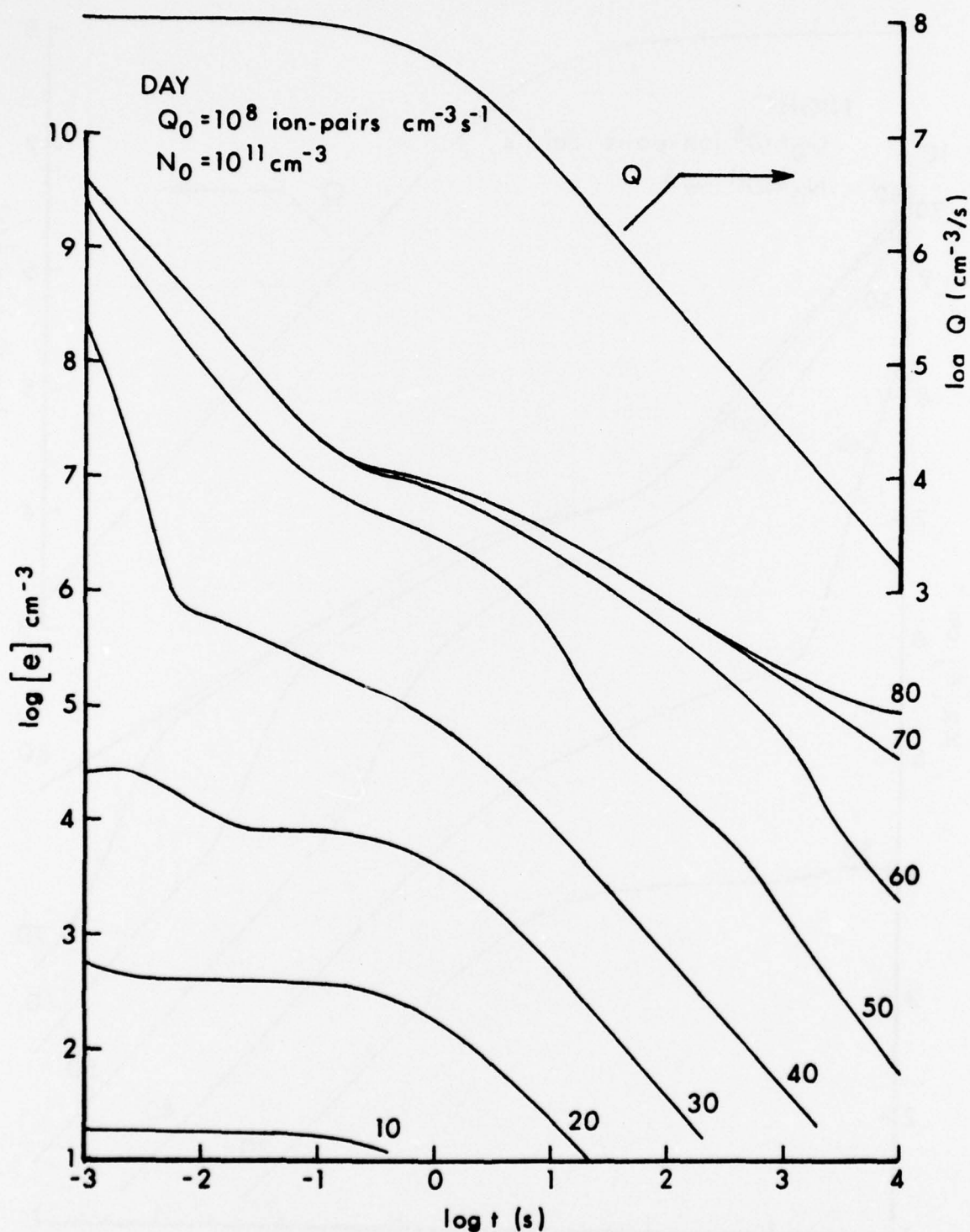


Figure 1. Logarithm of the computed daytime electron density vs. logarithm of time. Parameters are the altitudes in km. Top curve is the ion-pair production as a function of time.  $Q_0$  is the delayed ionization parameter, in ion pairs  $\text{cm}^{-3} \text{ s}^{-1}$ .  $N_0$  is prompt ionization parameter (electron density) in  $\text{cm}^{-3}$ .

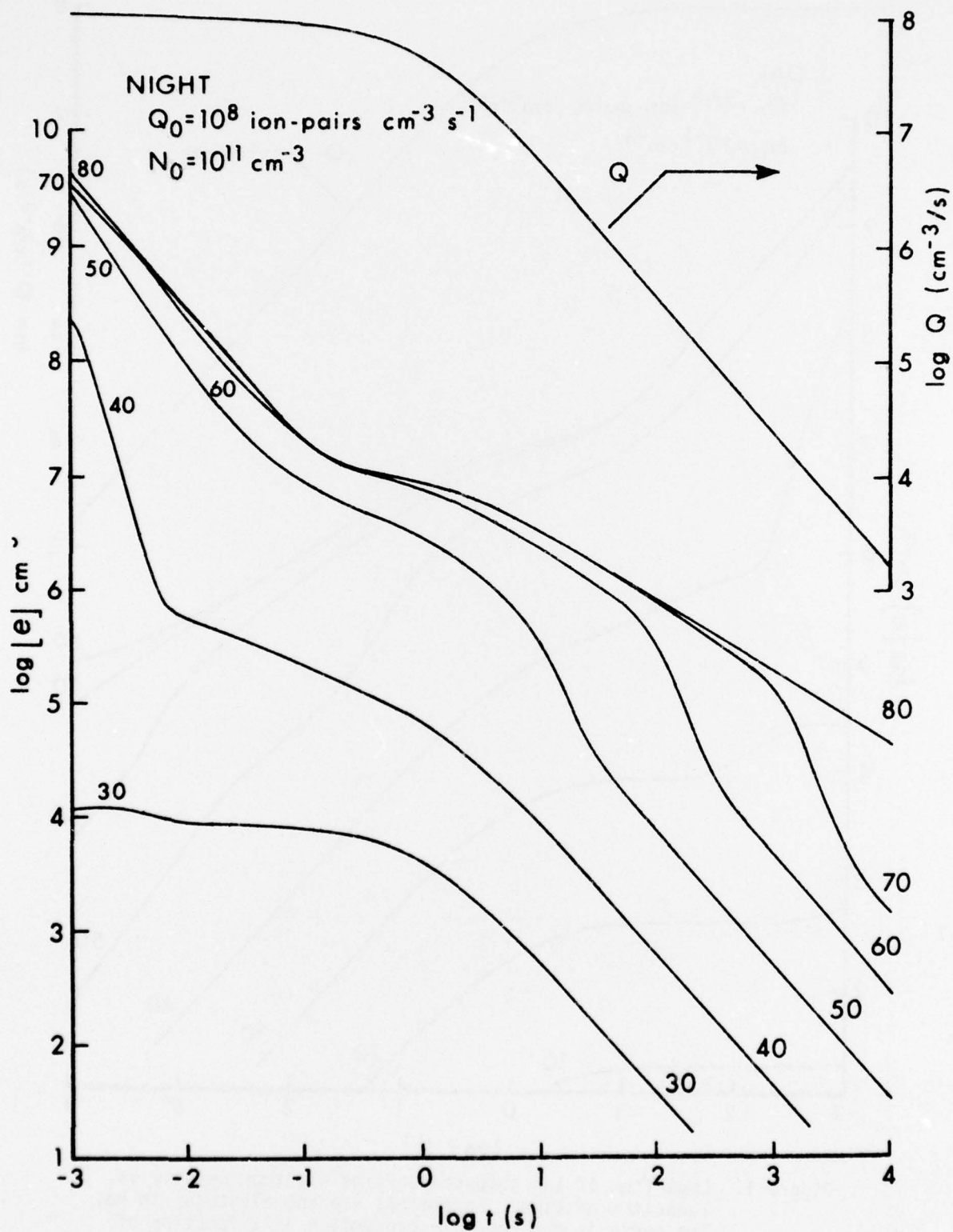


Figure 2. Same as Figure 1, except nighttime conditions.

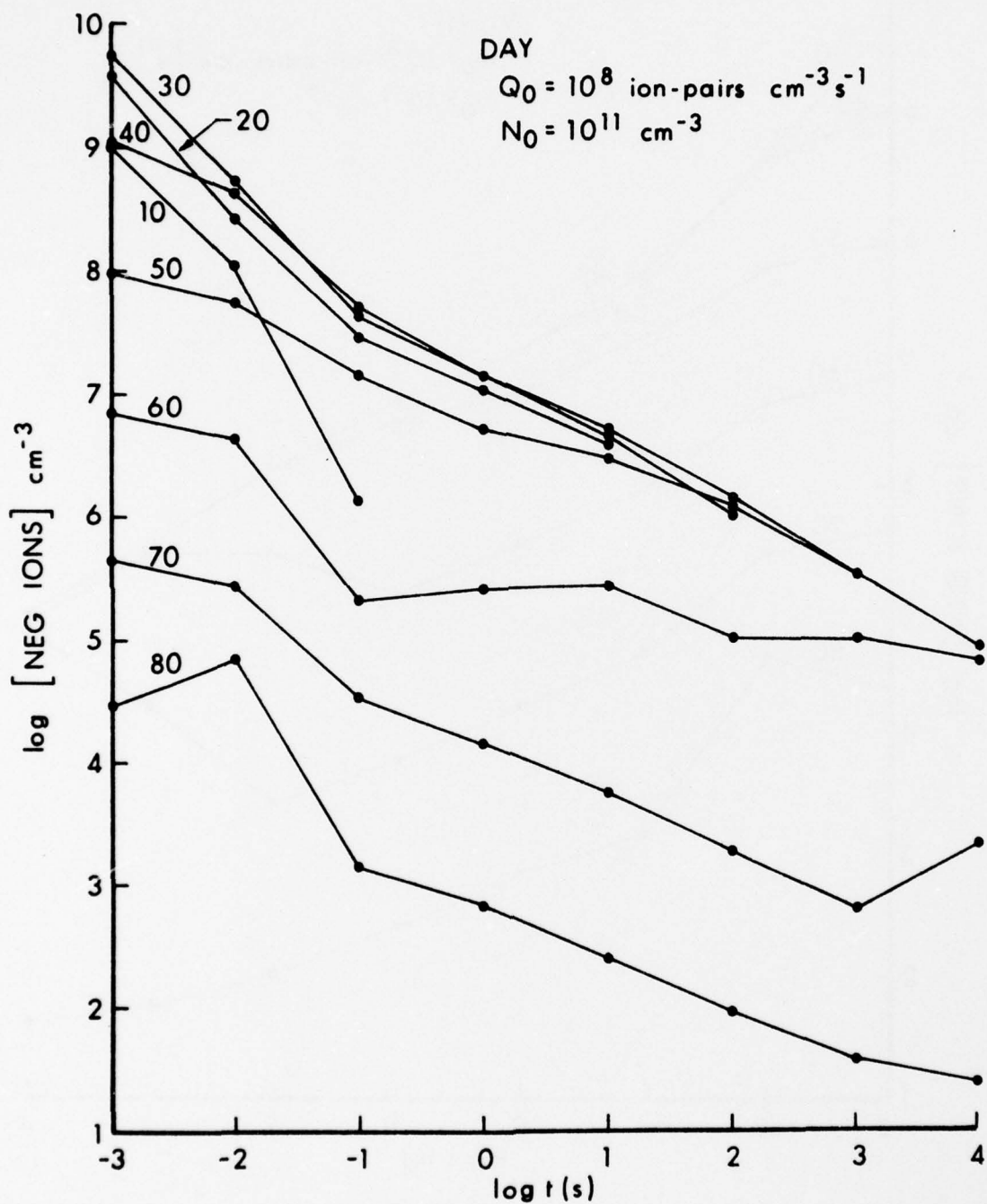


Figure 3. Logarithm of the sum of the computed negative ion densities vs. logarithm of time for daytime conditions. Parameters are the altitudes in km.



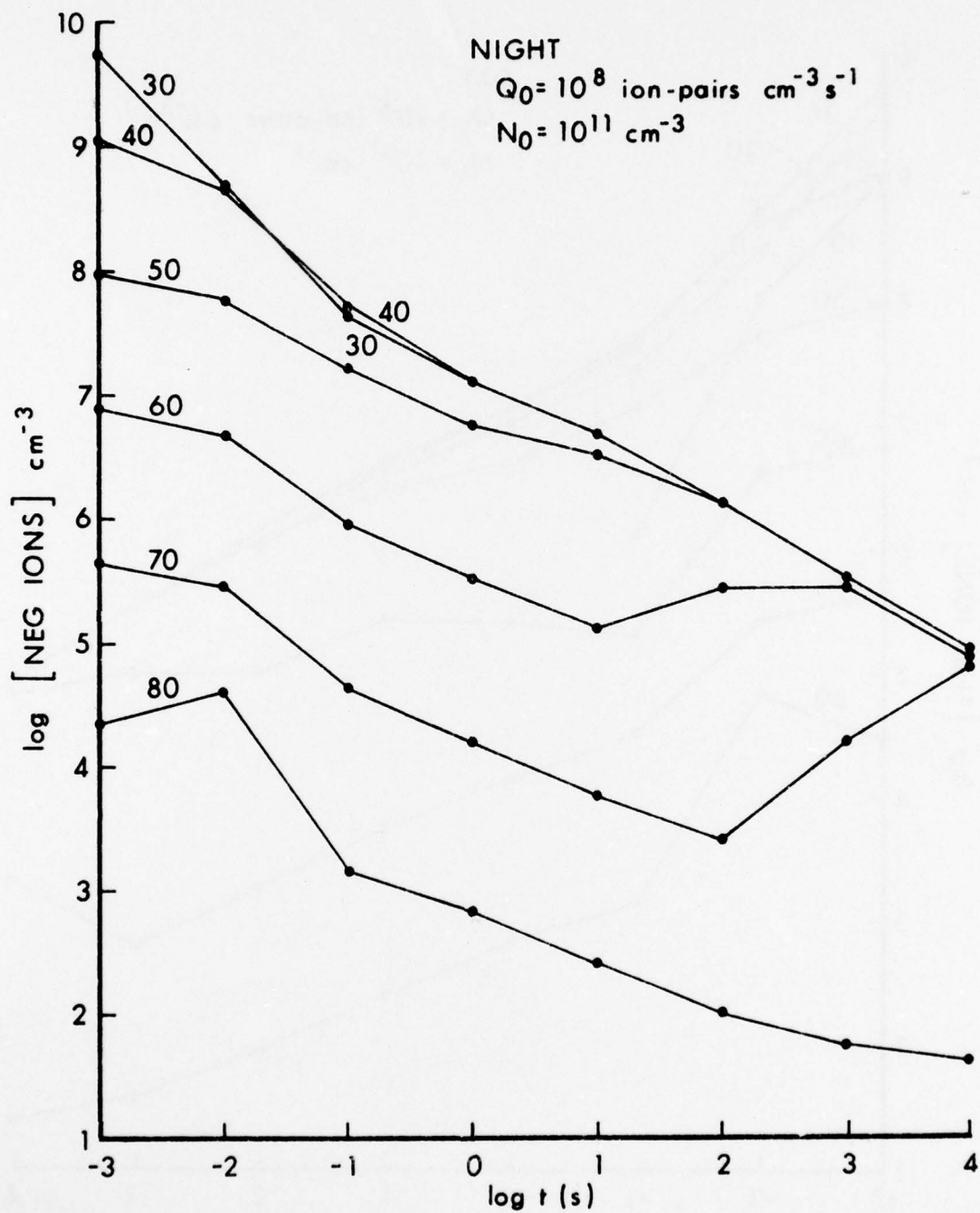


Figure 4. Same as Figure 3, except nighttime conditions.

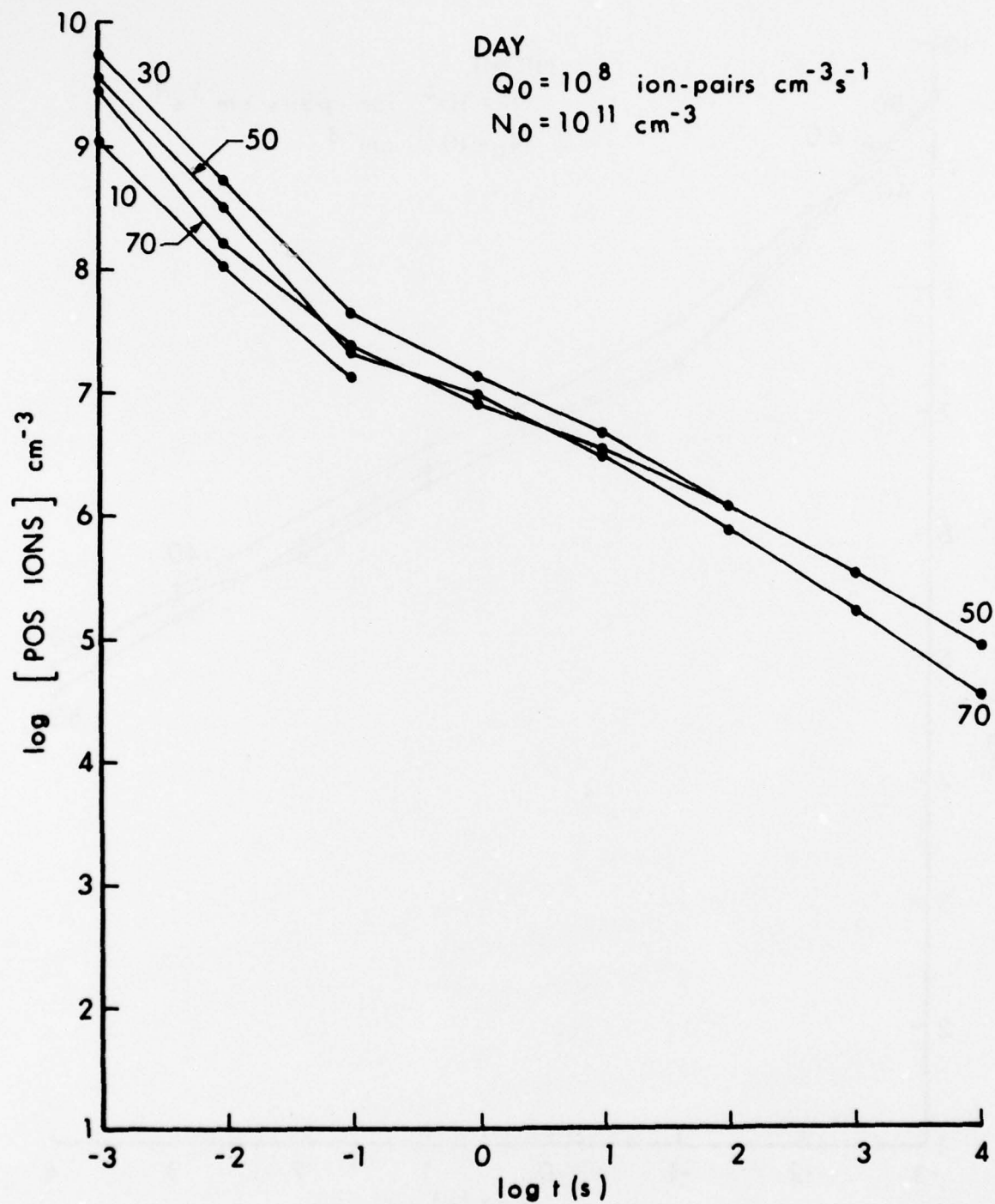


Figure 5. Logarithm of the sum of the computed daytime positive ion densities vs. logarithm of time. Parameters are the odd altitudes in km. (See text.)

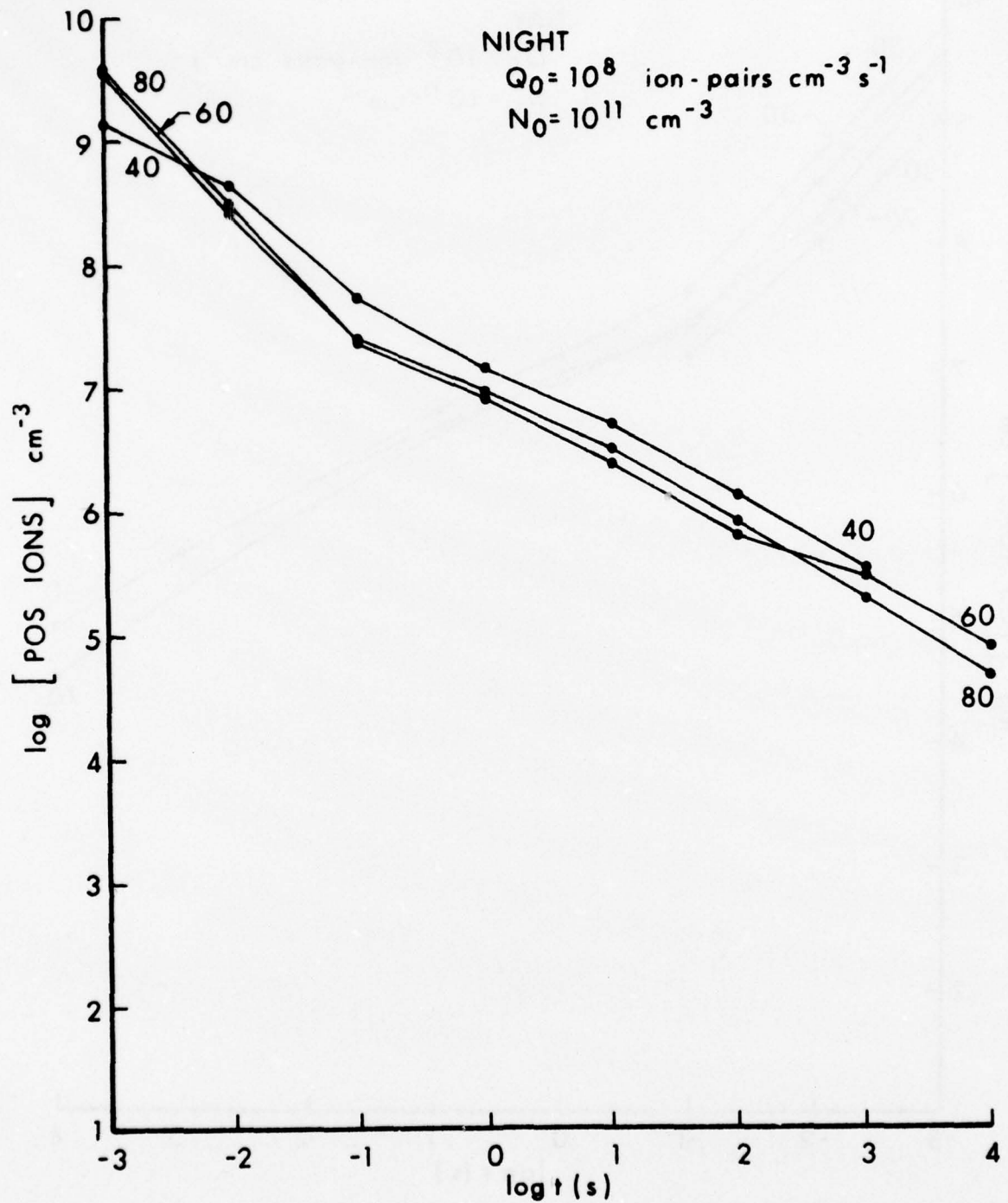


Figure 6. Same as Figure 5, except nighttime conditions for the even altitudes (See text).



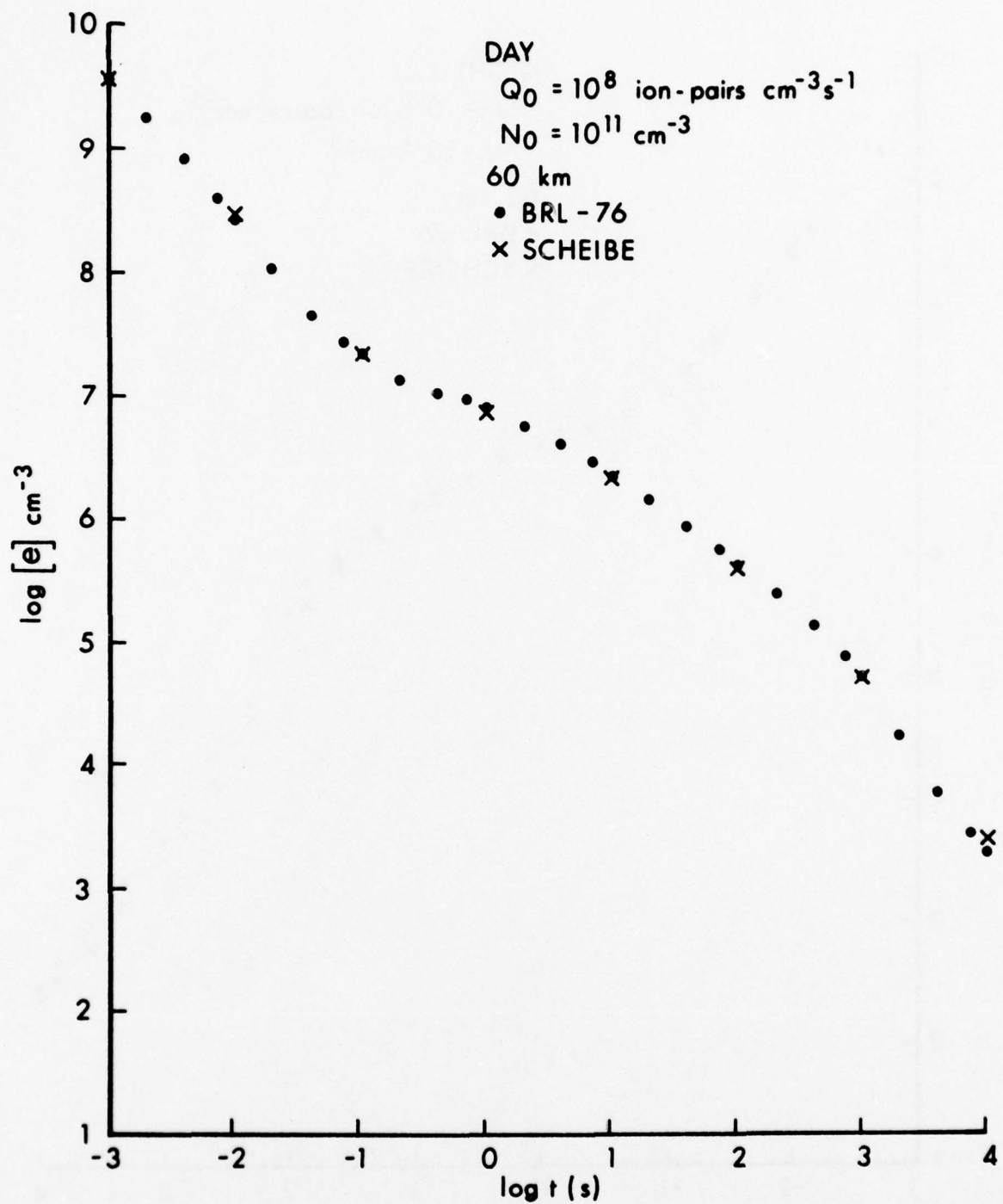


Figure 7. The daytime electron density, at 60 km, computed by BRL's BENCHMARK-76 code (•) and Scheibe's DAIRCHEM code (x).

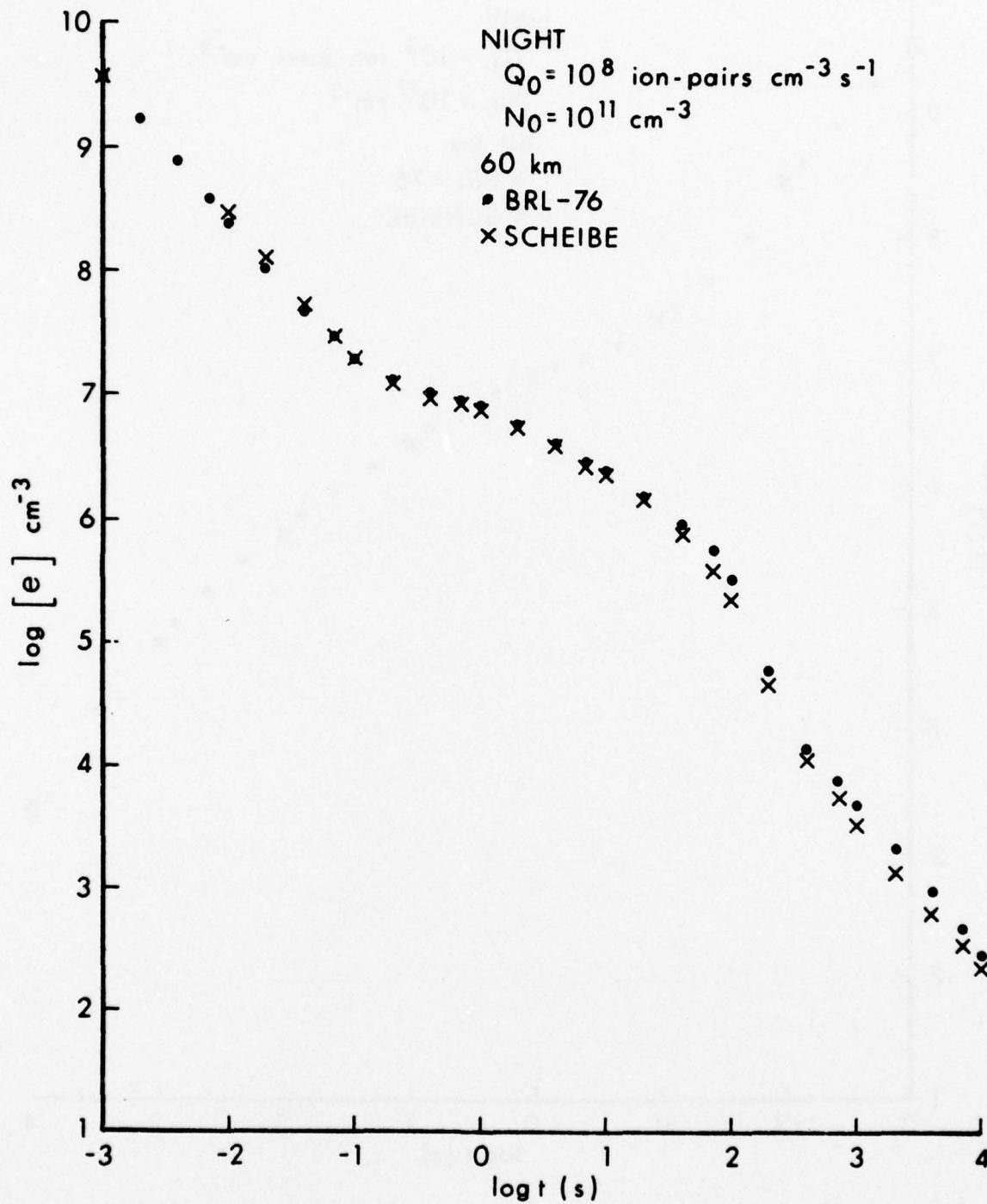


Figure 8. Same as Figure 7 except nighttime conditions.

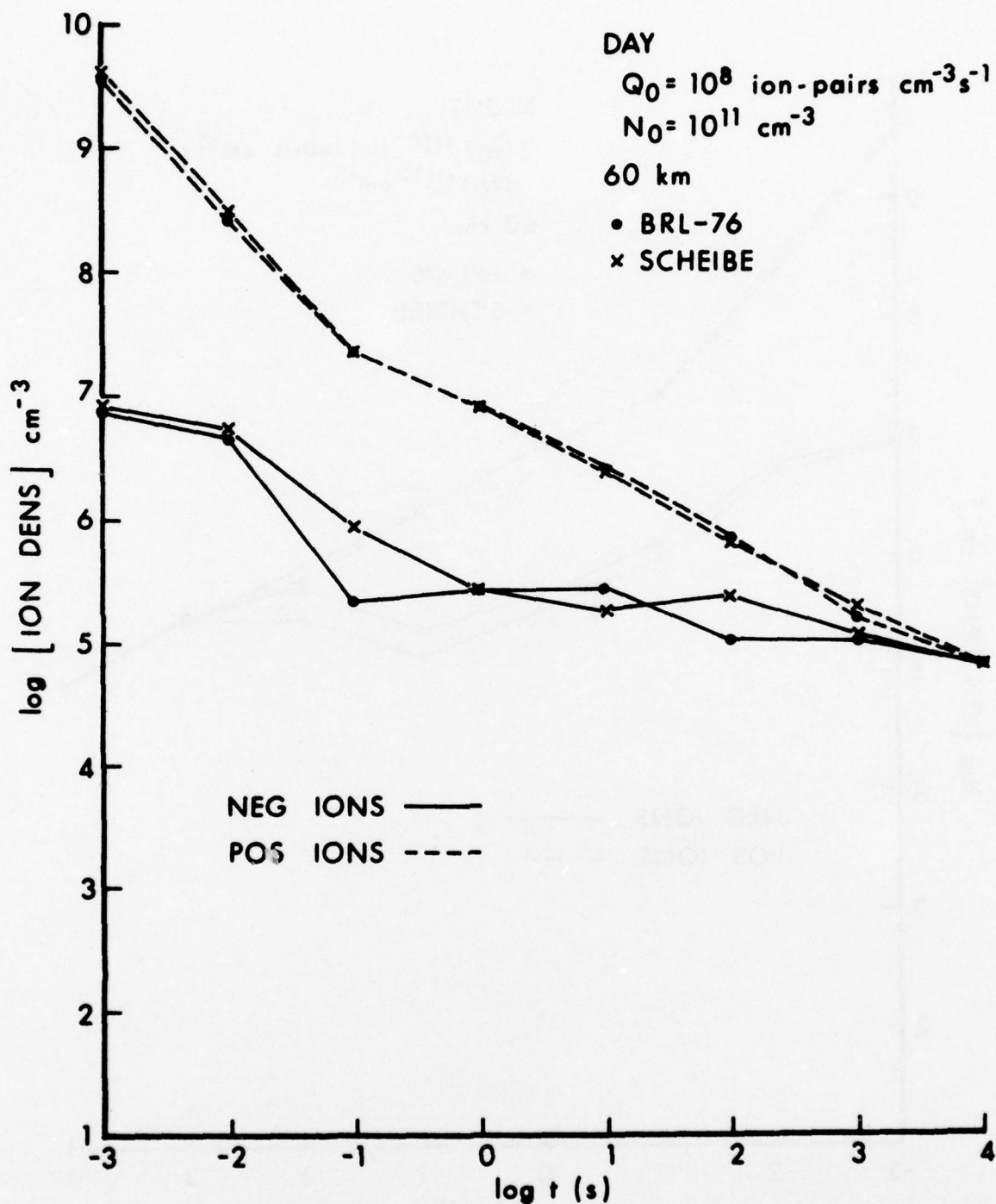


Figure 9. The total positive ion densities (---) and total negative ion densities (—) at 60 km for daytime conditions as computed by BRL's BENCHMARK-76 code (•) and Scheibe's DAIRCHEM code (x).



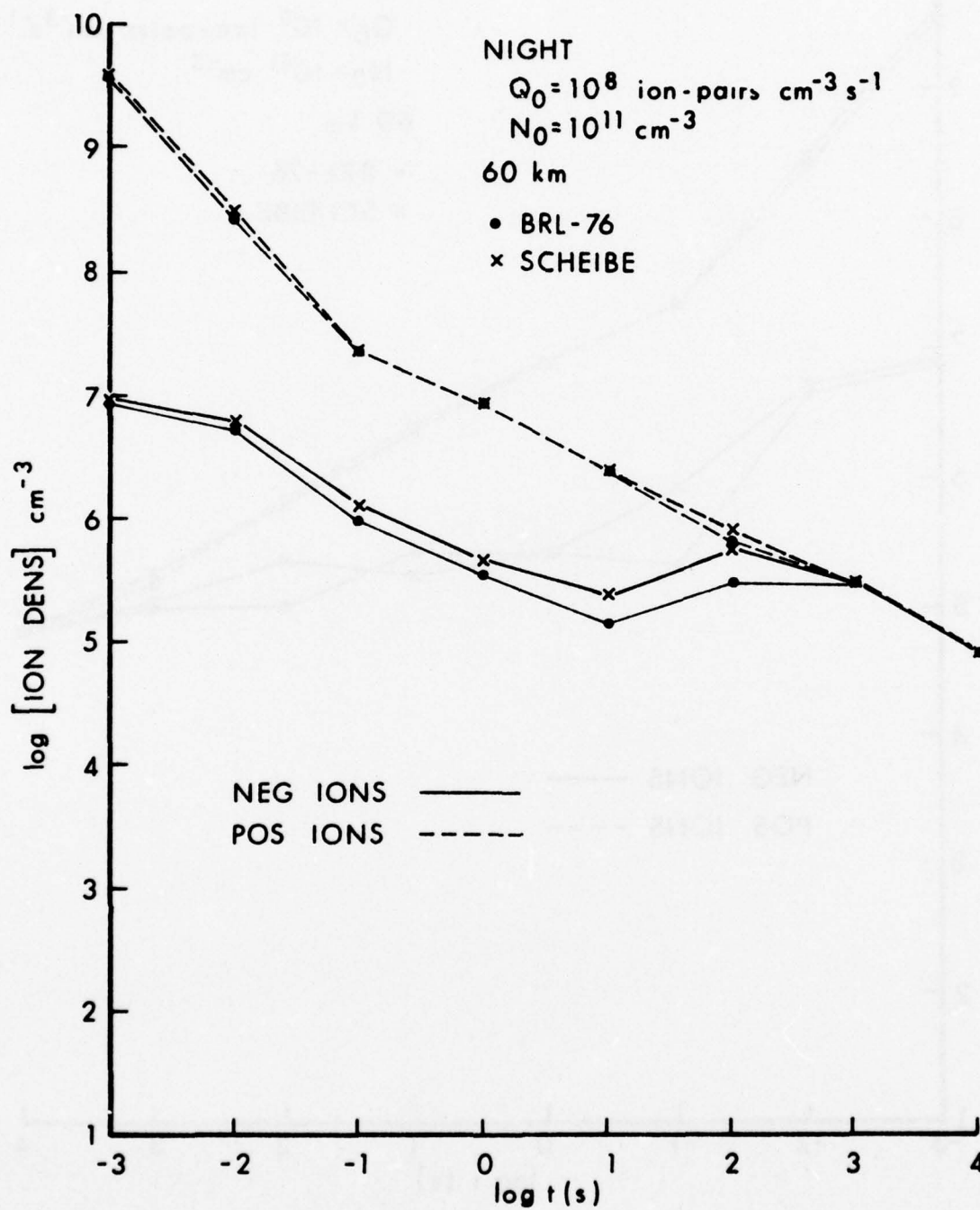


Figure 10. Same as Figure 9, except nighttime conditions.

### C. Sensitivity

Of the 210 ion-ion recombination reactions used in the BRL code only 8 have been measured in the laboratory. The remaining 202 were assigned a value of  $2.0 \times 10^{-7} (T/300)^{-1/2} \text{ cm}^3 \text{ s}^{-1}$ . Since there is some discussion, even as to the order of magnitude of some of the measured reactions, computations were made for the two cases wherein all of the ion-ion recombination rate coefficients,  $\alpha_i$ 's, are multiplied by  $10^{-1}$  and by  $10^{+1}$ . The results of this exercise, for nighttime conditions at an altitude of 60 km are shown in Figures 11, 12 and 13 for electrons negative ions, and positive ions, respectively. Though there are large changes in both the total positive ion and total negative ion densities, the change in the electron density barely exceeds a factor of two for a factor of 100 change in  $\alpha_i$ . This insensitivity to the precise value of rate coefficients can be expected whenever the production<sup>10</sup> of electrons is governed by the source term rather than the chemistry. For electrons it appears as though it is of the utmost importance to include the correct processes, rather than have very accurate rate coefficients. On the other hand, the hundredfold range of values assumed for the unmeasured ion-ion recombination coefficients can make substantial difference in the range of values computed for both the total negative ion and the total positive ion densities, as can be seen in Figures 12 and 13 respectively. We shall now show that a tenfold spread in each of these values is expected.

Whenever  $[N^-] \gg [e]$

$$\frac{d[N^-]}{dt} \approx q - \alpha_{\text{eff}}[N^-][N^+], \quad (2)$$

where  $q$  is the production of negative ions,  $\alpha_{\text{eff}}$  is the effective ion-ion

<sup>8</sup>D. Smith and M. J. Church, "Binary Ion-Ion Recombination Coefficients Determined in a Flowing Afterglow Plasma," Int. J. Mass Spec. and Ion. Phys. **19**, 185, 1976.

<sup>9</sup>For the case where selected  $\alpha_i$ 's are varied by the factors see "The Effects of Uncertainties in the Two-Body Ion-Ion Recombination Coefficient upon Computed Ion Distributions in the Stratosphere and Mesosphere," by J. M. Heimerl, BRL Report No. 1972, March 1977 (AD# A038263). Table 2 of this reference contains three typographical errors and one computational error. At 60 km the fourth reaction should read  $\text{H}^+(\text{H}_2\text{O})_3 + \text{NO}_3^-$ ; at 40 km the third reaction  $\text{H}^+(\text{H}_2\text{O})_4 + \text{CO}_3^-(\text{H}_2\text{O})$  and at 30 km the first reaction  $\text{H}^+(\text{H}_2\text{O})_4 + \text{CO}_3^-(\text{H}_2\text{O})$ . The values in Table 3 of this reference then correspond to variations in the corrected ion-ion recombination reactions listed in Table 2. The computations at 40 km should have been carried out with  $\text{H}^+(\text{H}_2\text{O})_4 + \text{NO}_3^-(\text{H}_2\text{O})$  as the second reaction. Recomputation shows some changes in the percentages in Table 3 but the conclusions therein remain unchanged.

<sup>10</sup>For a counter example wherein chemistry dominates the production term, see F. E. Niles, "Electron Density in the Beta Patch Following a Spartan Burst," BRL Report No. 1518, December 1970, Figure 9. (AD# 879464)

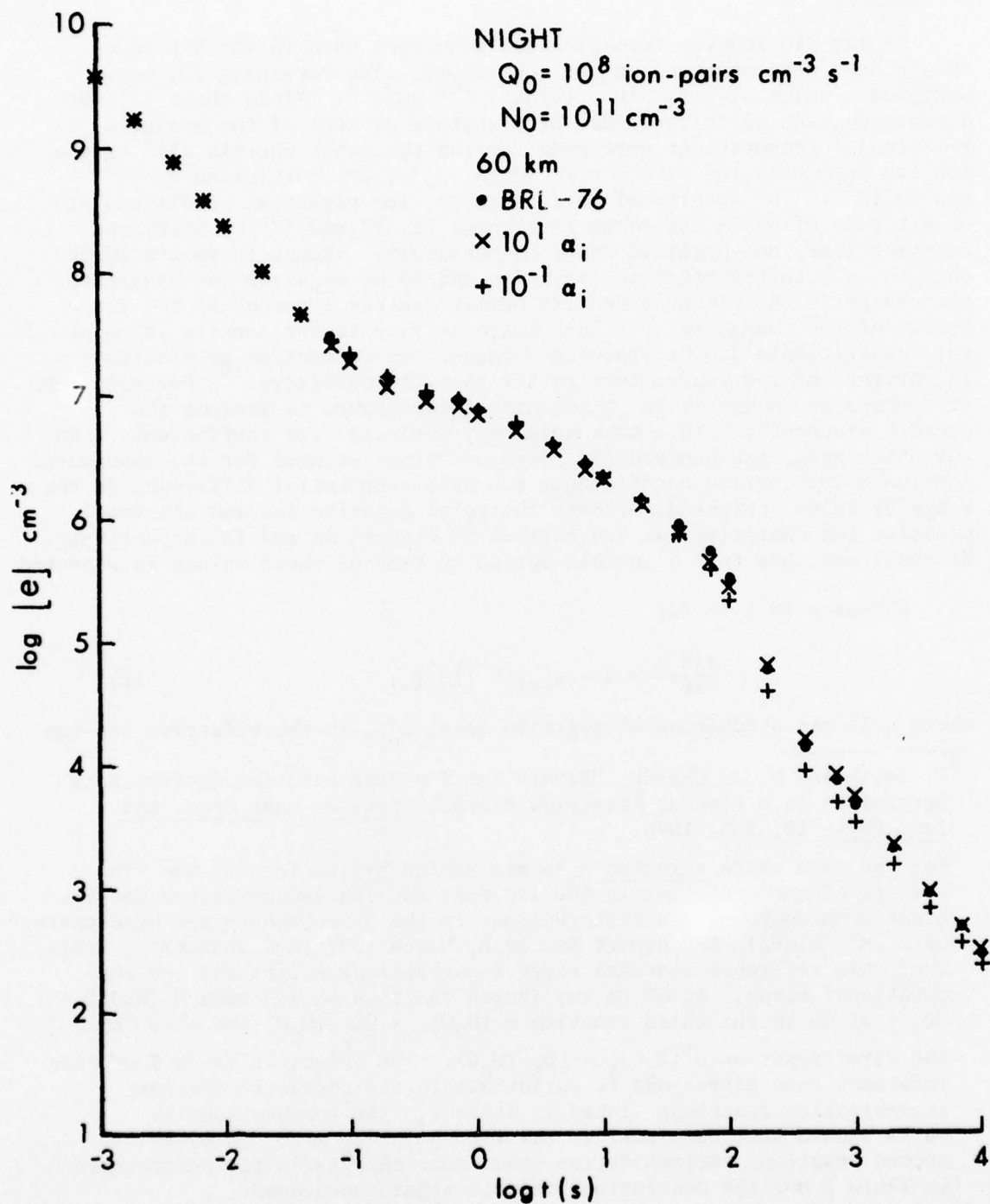


Figure 11. Sensitivity of the computed nighttime electron density at 60 km to simultaneous decade variations in each value of the 210 ion-ion recombination coefficients used in the BENCHMARK-76 code.

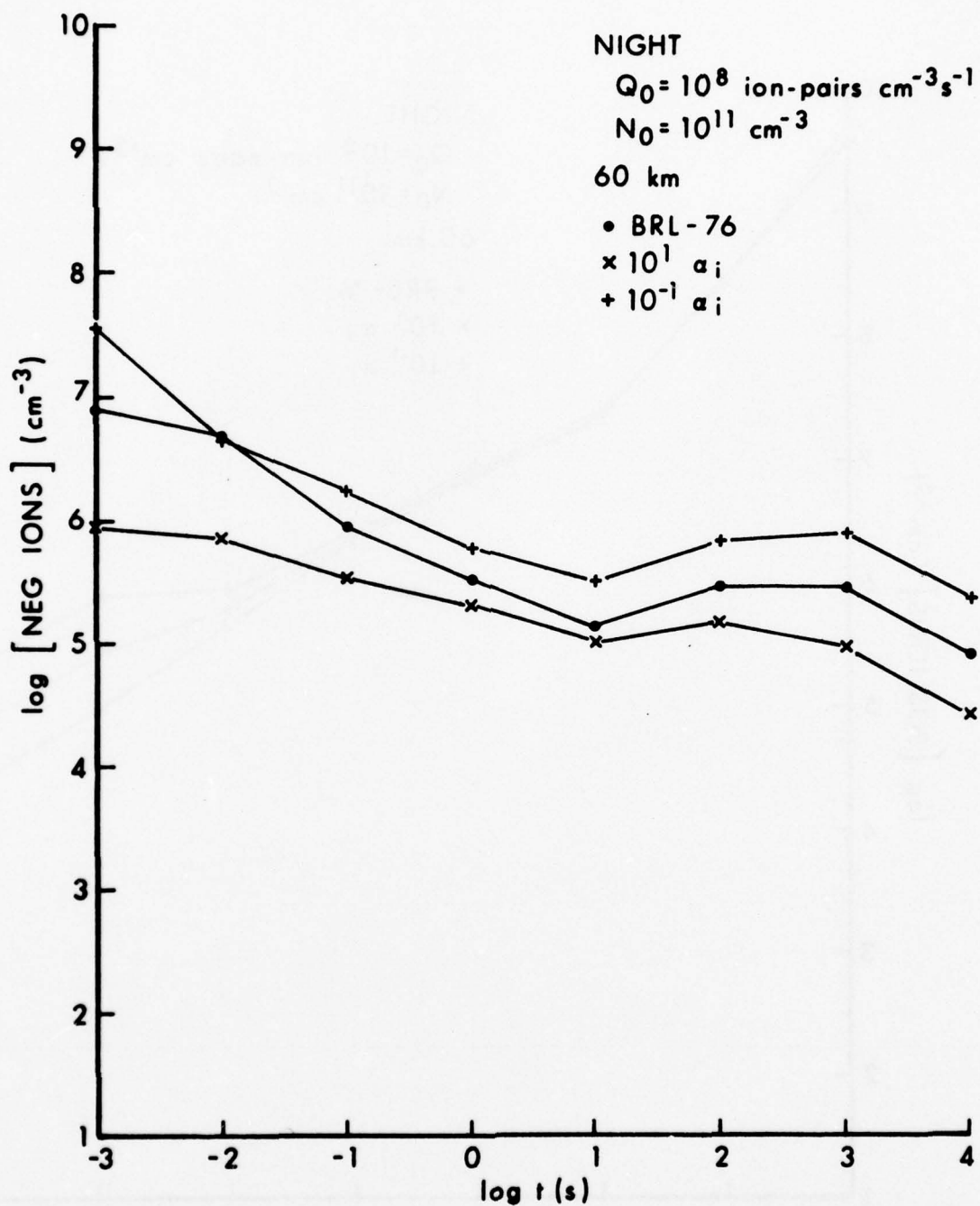


Figure 12. Sensitivity of the computed nighttime total negative ion density for the conditions stated in Figure 11.



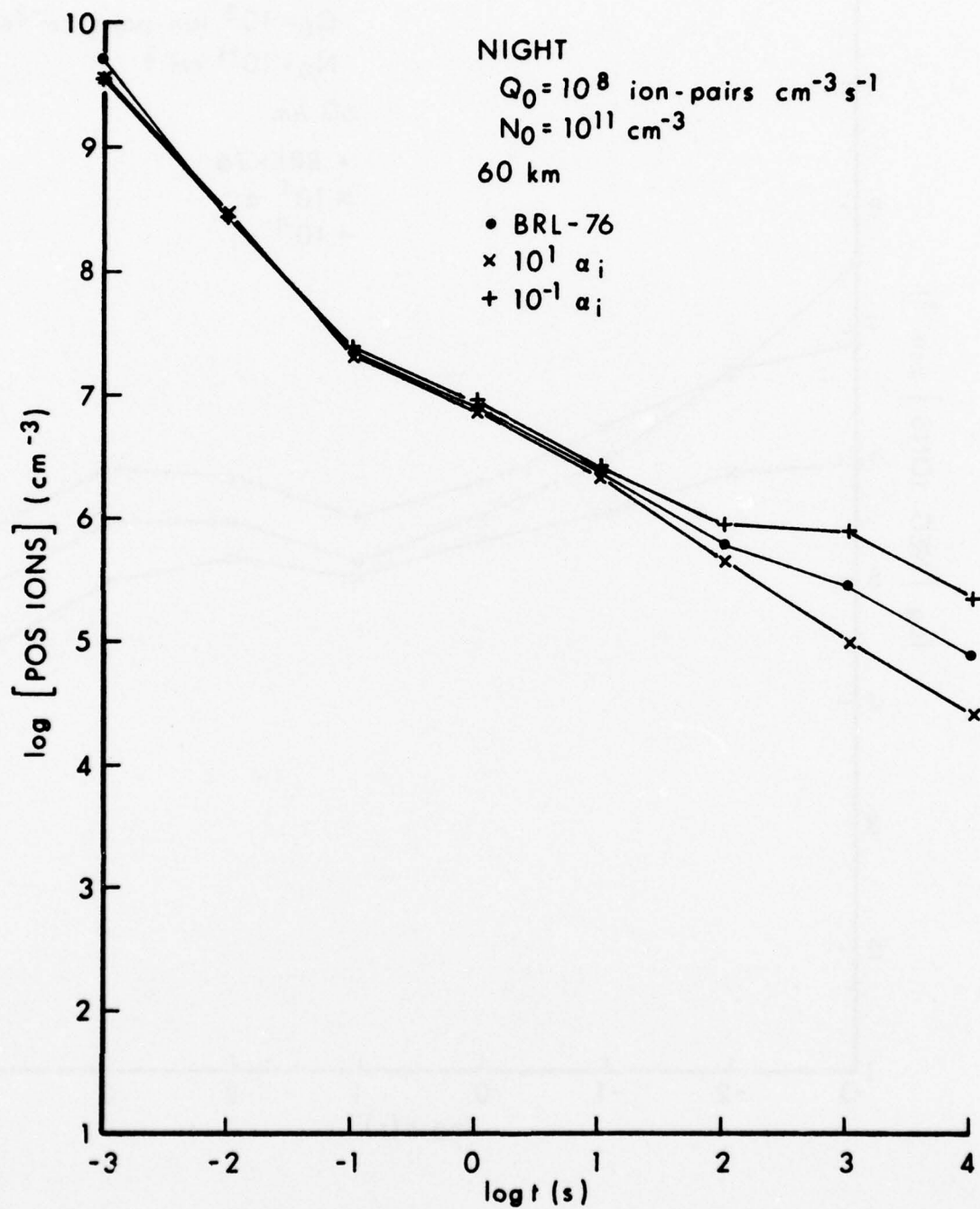


Figure 13. Sensitivity of the computed nighttime total positive ion density for the conditions stated in Figure 11.

recombination coefficient and  $[N^-]$  and  $[N^+]$  are the total negative and total positive ion densities, respectively. Under steady-state conditions, i.e.,  $d[N^-]/dt = 0$ , and whenever  $[N^-] \approx [N^+]$ , equation (2) reduces to

$$q \approx \alpha_{\text{eff}} [N^+]^2 \quad \text{or} \quad (3a)$$

$$q \approx \alpha_{\text{eff}} [N^-]^2 \quad (3b)$$

For the results shown in Figures 12 and 13 the production of negative ions remains unaltered and so  $q = \text{constant}$ . Since  $\alpha_{\text{eff}} \propto \sum \alpha_i$  a factor of 100 change in every  $\alpha_i$  is reflected as a factor of 100 change in  $\alpha_{\text{eff}}$ . For such a change equations (3a) and (3b) show that both  $[N^+]$  and  $[N^-]$  will change by a factor of ten.

This factor of ten is observed at the latest times in Figures 12 and 13 because the conditions under which this factor applies, i.e.,  $[N^-] \gg [e]$ ,  $[N^-] \approx [N^+]$  and steady state, are all found when  $t \geq 10^3$  s. (Compare Figures 11 and 12 and Figures 12 and 13. In Section D we shall find that the steady state condition is reached by about one second.)

#### D. Equivalent Rate Coefficients

Once the individual species concentrations have been computed as a function of time and altitude a set of equivalent rate coefficients, ERC's, can be generated.

The effective electron-ion recombination coefficient is defined by

$$\alpha_d = \Sigma R_{ei} / [e] \Sigma [N_k^+] \quad (4)$$

where  $\Sigma R_{ei}$  is the sum of the rates for electron-ion recombination,  $[e]$  the electron density and  $[N_k^+]$  is the density of the  $k^{\text{th}}$  positive ion species. This sum is over all positive ion species.

There are 24 reactions<sup>11</sup> that make up the  $\Sigma R_{ei}$  of Equation (4). A sufficient number of reactions is carried in the model so that, except for  $N^+$ ,  $O^+$  and  $O_2^+(N_2)$ , each positive ion species reacts with an electron. (The two products of the  $NO^+ + e$  reaction, viz.  $N(^4S)$  and  $N(^2D)$ , are carried explicitly as two separate reactions.)

Figures 14 and 15 show the temporal variation of  $\alpha_d$  for daytime and nighttime conditions, respectively. The numbers on the curves refer to altitude,  $z$ , in kilometers. For the lower altitudes  $\alpha_d$  approaches limiting values determined by the relative composition of cluster ions and their respective electron-ion recombination coefficients. At the higher altitudes the limiting values of  $\alpha_d$  are not yet attained, even after  $10^4$  model seconds.

<sup>11</sup>Reactions 138-162 inclusive; see Appendix for reaction list.

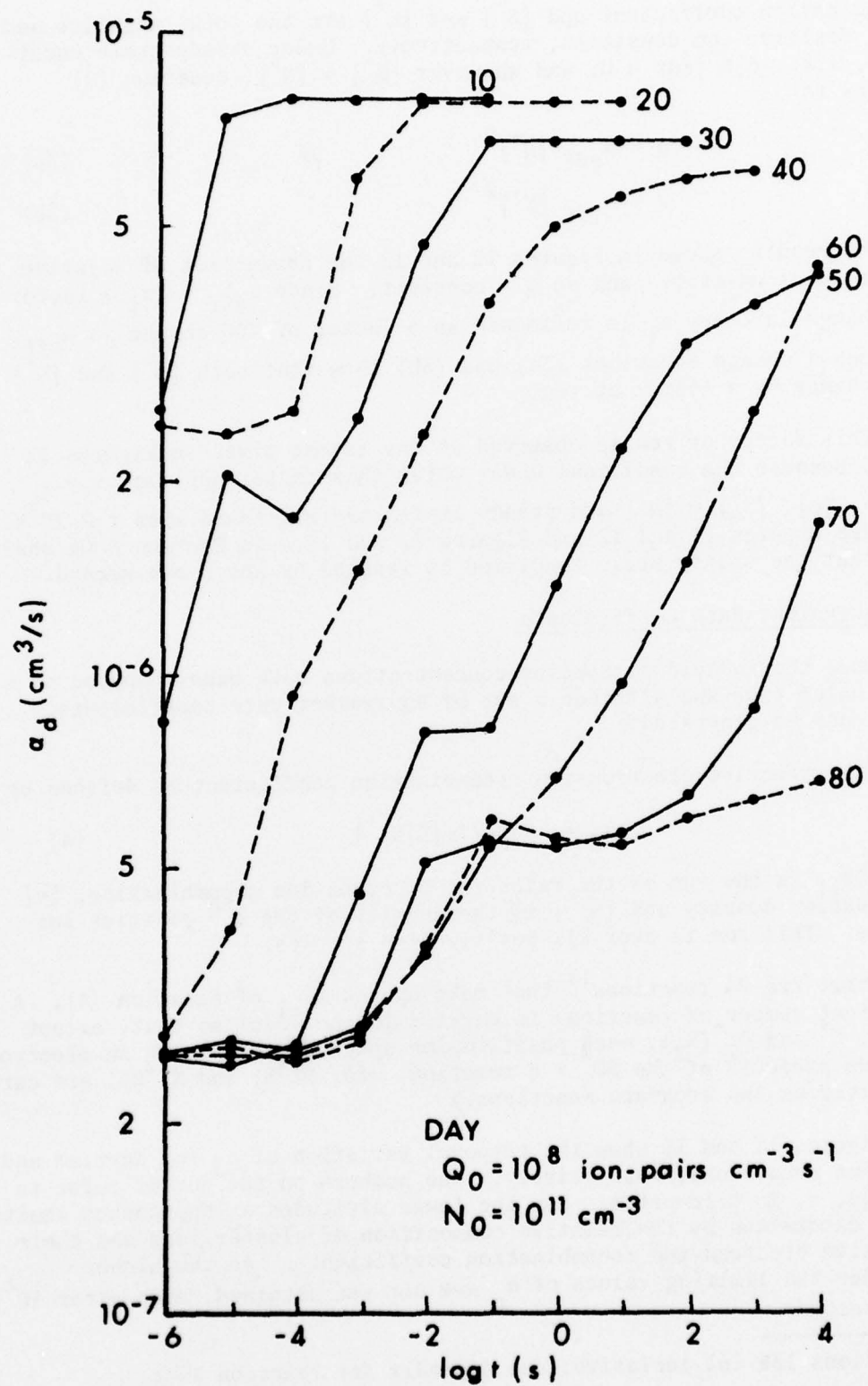


Figure 14. Effective electron-ion recombination rate coefficient,  $\alpha_d$ , as a function of time for daytime conditions. Parameters are the altitudes in km.

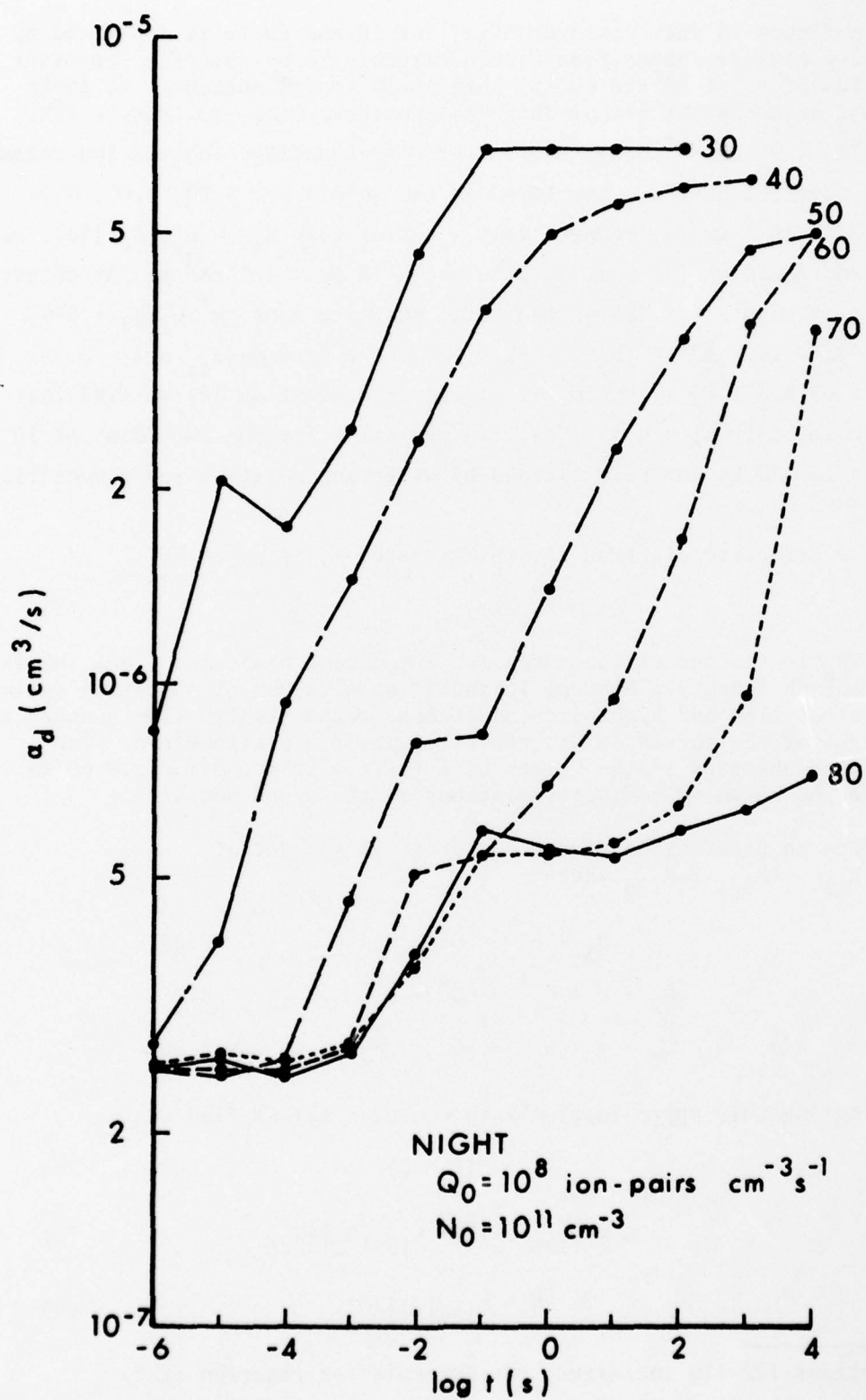


Figure 15. Same as Figure 14, except nighttime conditions.



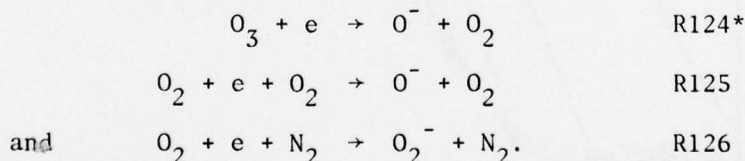
In figure 14 the crossover of  $\alpha_d$  for 50 and 60 km is explained by differing cluster composition with altitude. To be specific, consider the value of  $\alpha_d$  at 50 and 60 km, both at  $10^4$  model seconds. At 50 km  $H^+(H_2O)_3$  accounts for 64% of the total positive ions,  $NO^+(H_2O)$  - 20%,  $NO^+(H_2O)_2$  - 9% and  $H^+(H_2O)_4$  - 8%. The corresponding electron ion-recombination coefficients,  $\alpha_{ei}$ , employed in the code are: 5.20, 1.02, 2.04 and  $6.22 \times 10^{-6} \text{ cm}^3/\text{s}$ , respectively. Noting that  $R_{ei} = \alpha_{ei} [N_k^+][e]$ , we find from Equation (4) that  $\alpha_d(z=50 \text{ km}, t=10^4 \text{ s}) = 4.2 \text{ cm}^3/\text{s}$ . At 60 km,  $H^+(H_2O)_3$  accounts for 40% of the total positive ions,  $H^+(H_2O)_4$  - 26%,  $NO^+(H_2O)_2$  - 24% and  $NO^+(H_2O)$  - 9%. The corresponding  $\alpha_{ei}$  are: 5.29, 6.33, 2.08 and  $1.04 \times 10^{-6} \text{ cm}^3/\text{s}$ . Again from Equation (4) we find that  $\alpha_d(z=60 \text{ km}, t=10^4 \text{ s}) = 4.4 \text{ cm}^3/\text{s}$ . In a similar fashion the "dip" at  $10^{-4}$  seconds for 30 km can be explained by differing positive-ion composition with time.

The effective electron attachment rate, A, is given by

$$A = \Sigma R_A / [e] \quad (5)$$

where  $\Sigma R_A$  is the sum of the rates for attachment processes<sup>12</sup> and  $[e]$  is the electron density. Figures 16 and 17 show values of A plotted against time for daytime and nighttime conditions, respectively. The numbers to the right of the curves denote the altitude, z, in kilometers. The variations observed in the values of A for  $t \geq 10^4 \text{ s}$  and for  $z \geq 60 \text{ km}$  will now be shown to reflect variations in the ozone density.

From an examination of the output it is found that  $\Sigma R_A \approx R_{124} + R_{125} + R_{126}$  where



Substituting this approximation into equation (5) we find that

$$A \approx C(1 + B) \quad (6)$$

$$\text{where } C = k_{125}[O_2]^2 + k_{126}[O_2][N_2] \quad (7)$$

$$\text{and } B = k_{124}[O_3]/C \quad (8)$$

<sup>12</sup>Reactions 122-126 inclusive; see Appendix for reaction list.

\* Read as Reaction 124. A complete listing of reactions and references may be found in the Appendix.

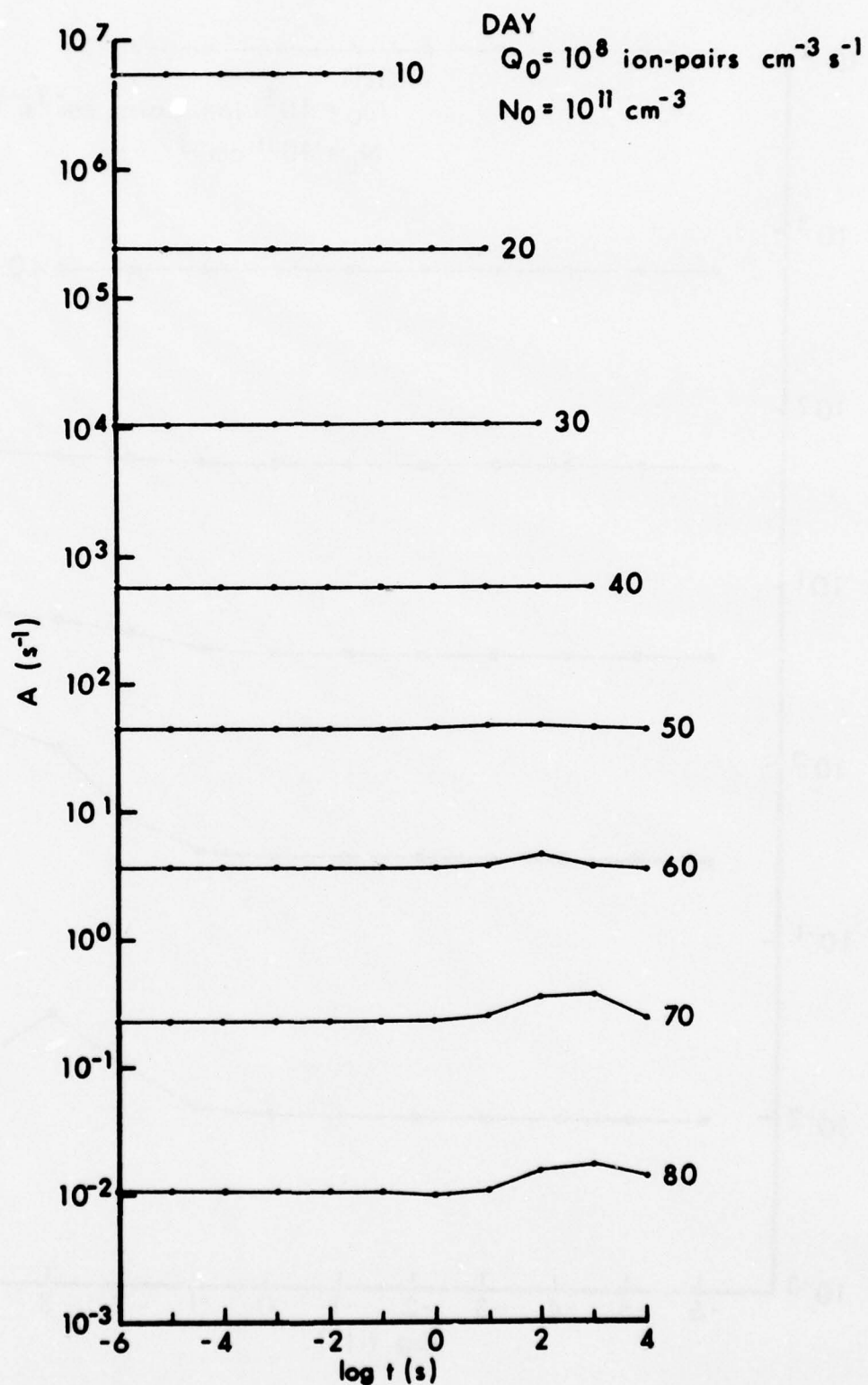


Figure 16. Effective electron attachment coefficient,  $A$ , as a function of time for daytime conditions. Parameters are the altitudes in km.

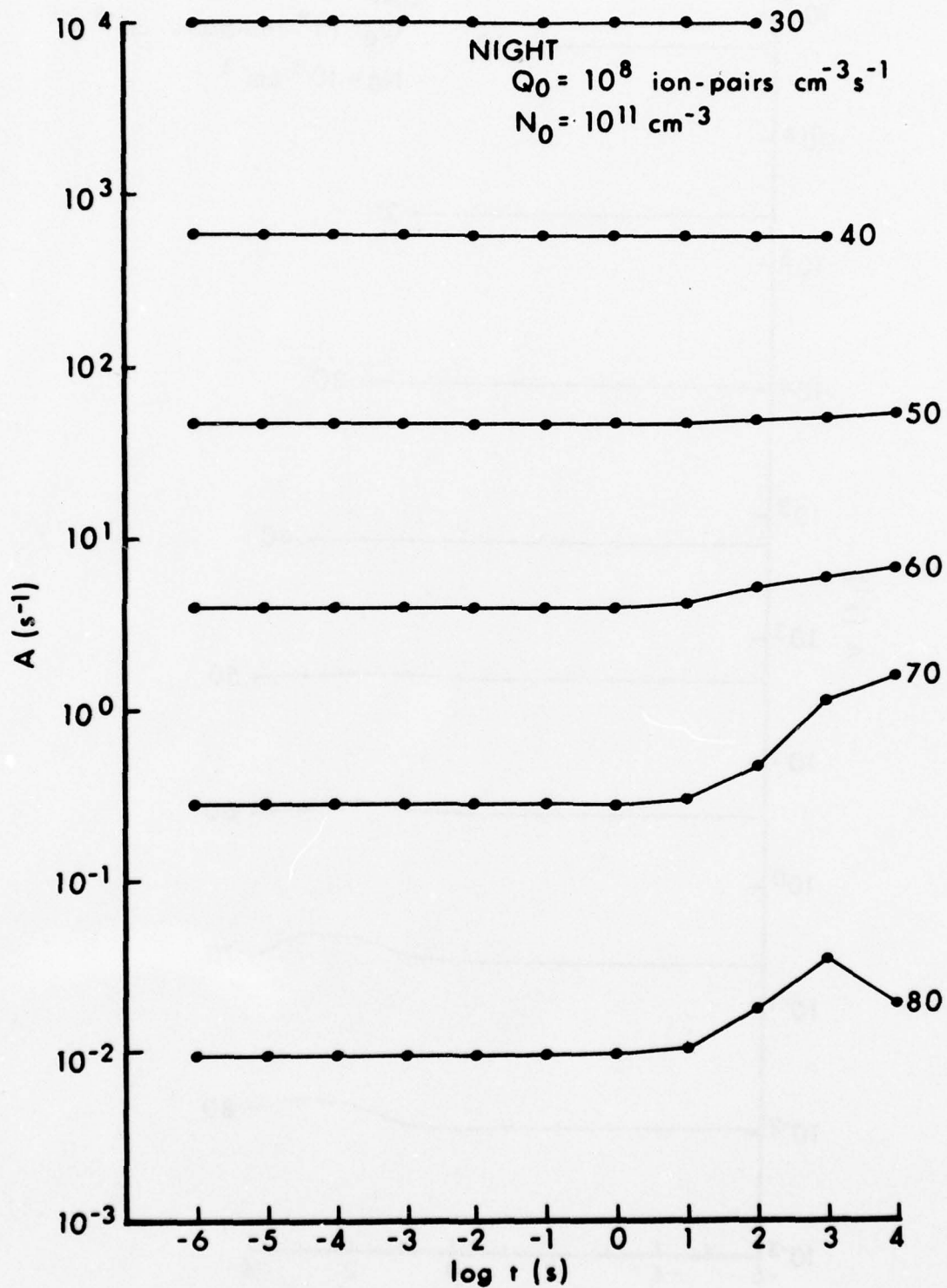


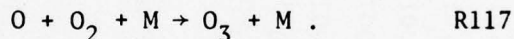
Figure 17. Same as Figure 16, except nighttime conditions.

For a given altitude,  $C$  defined by equation (7) is approximately constant. Since, again at a given altitude, the value of  $k_{124}$  is fixed,  $B$  in equation (8) reflects the changes in  $[O_3]$ . This reflection shows up in the expression for  $A$ , equation (6).

The value of  $B$  in equation (8) defines the importance of reaction 124 relative to the three-body attachment reactions, i.e.  $B = R_{124} / (R_{125} + R_{126})$ . Tables 1 and 2 show the values of  $B$  for daytime and nighttime conditions, respectively. From Table 2 we find that  $B$  is small or constant in time, or both (1) for altitudes of 50 km or less over the entire time interval studied or (2) for the altitude region 60-80 km and for  $t \leq 10^0$ s. From equation (6) we expect the value of  $A$  to be constant in time for these conditions and this is observed in Figure 17. For the altitude region 60-80 km and for  $t \geq 10^1$ s the values of  $B$  in Table 2 are seen to vary with time. The corresponding variations in  $A$  are again found in Figure 17.

A similar analysis follows for the values of  $B$  for daytime conditions given in Table 1.

We will now briefly and qualitatively examine the proximate cause of the  $[O_3]$  variations. An examination of the output reveals that for the higher altitudes by  $t = 10^{-1}$ s the production of  $[O_3]$  is almost entirely due to the reaction



This reaction shows that at a given altitude, i.e. both  $[O_2]$  and  $[M]$  are constants, the ozone production will track the atomic oxygen density. The  $[O]$  is found to be constant for times up to  $10^0$ s at the higher altitudes; thus  $[O_3]$  production is approximately constant. The ozone density can rise, however, because the net loss rate of ozone due to reactions with:  $H$ ,  $N$ ,  $NO$ ,  $O$ ,  $O(^1D)$ ,  $O_2(^1\Sigma)$  and electrons (corresponding to reactions 70, 81, 88, 93, 94, 100, 104 and 124, respectively) falls. These higher  $[O_3]$  values are not maintained, because by  $10^0$ s the atomic oxygen density declines leading to the eventual decline in  $[O_3]$ .

The effective electron detachment rate is defined by

$$D = \Sigma R_D / \Sigma [N_k^-], \quad (9)$$

where the  $R_D$  are the rates for individual detachment processes and  $[N_k^-]$  is the  $k^{\text{th}}$  negative ion density. The sums are over all detachment rates and all negative ion densities, respectively. The two detachment processes considered in the code are photodetachment and two-body collisional detachment; the former is a set of six reactions and the latter eleven.<sup>13</sup>

<sup>13</sup>Reactions 1-5 and 11 for photodetachment; 127-137 inclusive for two body collisional detachment; see Appendix for reaction list.



TABLE 1. VALUES OF B FOR DAYTIME CONDITIONS

z (km)	t(s)	10 <sup>-6</sup>	10 <sup>-5</sup>	10 <sup>-4</sup>	10 <sup>-3</sup>	10 <sup>-2</sup>	10 <sup>-1</sup>	10 <sup>0</sup>	10 <sup>1</sup>	10 <sup>2</sup>	10 <sup>3</sup>	10 <sup>4</sup>
80	0.16	0.16	0.16	0.16	0.16	0.16	0.15	0.11	0.17	0.64	0.74	0.51
70	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.10	0.52	0.58	0.07
60	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.07	0.76	0.06	0.01
50	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.05	0.06	0.03	.004
40	.007	.007	.007	.007	.007	.007	.008	0.01	0.01	0.01	.008	-
30	.001	.001	.001	.001	.001	.002	.002	.002	.002	.002	-	-
20	10 <sup>-4</sup>	10 <sup>-4</sup>	10 <sup>-4</sup>	10 <sup>-4</sup>	10 <sup>-4</sup>	10 <sup>-4</sup>	10 <sup>-4</sup>	10 <sup>-4</sup>	10 <sup>-4</sup>	-	-	-
10	10 <sup>-6</sup>	10 <sup>-6</sup>	10 <sup>-6</sup>	10 <sup>-6</sup>	10 <sup>-6</sup>	10 <sup>-6</sup>	10 <sup>-6</sup>	-	-	-	-	-

TABLE 2. VALUES OF B FOR NIGHTTIME CONDITIONS

80	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.03	0.12	1.00	2.73	1.10
70	0.21	0.21	0.21	0.21	0.21	0.21	0.21	0.19	0.26	0.99	3.99	3.40
60	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.12	0.41	0.48	0.47
50	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.06	0.09	0.08	0.08
40	.007	.007	.007	.007	.007	.007	.008	0.01	0.01	0.01	0.01	-
30	.001	.001	.001	.001	.002	.002	.002	.002	.002	.002	-	-

Figures 18 and 19 show D vs time for daytime and nighttime conditions, respectively. Altitudes, in kilometers, are listed nearby their corresponding curves. In both figures the most notable feature is that no curve attains a constant value at late times. ("Late time" for the 10 km case is  $10^{-1}$  s.) A detachment process that is important at all the altitudes studied is



This reaction has been assigned the upper limit of  $1 \times 10^{-12} \text{ cm}^3/\text{s}$ .<sup>14</sup> To examine the effect this value might have on the effective electron detachment rate we assigned a value of  $1 \times 10^{-14} \text{ cm}^3/\text{s}$ <sup>15</sup> and exercised the model over the altitude range 50-80 km for daytime conditions. Table 3 shows the comparison of the values of D as a function of time. Since  $R_{129} \propto k_{129}$ , equation (9) predicts that values of D should be greater the larger the value of  $k_{129}$ . This behavior is observed in Table 3. As may be seen in this table the percentage differences in the value of D in some cases amounts to about 50% for a hundredfold change in the value of  $k_{129}$ . Another result of this exercise was that while reaction (129) was no longer dominant, it was still significant and could not in general be ignored.

The effective recombination coefficient,  $\psi$ , is defined by

$$\psi = (1 + \lambda)(\alpha_d + \lambda\alpha_i), \quad (10)$$

where  $\lambda$  is the ratio of the total negative ion density to the electron density (other terms have been defined). In the steady state, a criterion many times employed in hybrid models,<sup>16</sup>  $\psi$  should equal the source term divided by the square of the electron density,  $Q/[e]^2$ . At a given altitude, the value of  $\psi$  (solid line in Figure 20), and the value of  $Q/[e]^2$  (dashed line in Figure 20) are about equal (i.e., within about 20%) for times greater than about one second (see arrow). This result also holds true for daytime conditions (not shown).

#### E. Example of Detailed Analysis

In this section we shall illustrate the type of detailed analysis available from the BENCHMARK-76 program output. In Figure 1 the electron density at 80 km does not follow the source term, Q, at late times, but actually begins to increase. This is explained, as we shall see, by an additional source for electrons.

<sup>14</sup>W. Lindinger, D. L. Albritton, F. C. Fehsenfeld and E. E. Ferguson, "Reactions of  $O^-$  with  $N_2$ ,  $N_2O$ ,  $SO_2$ ,  $NH_3$ ,  $CH_4$  and  $C_2H_4$  and  $C_2H_2^-$  with O from 300°K to relative kinetic energies of  $\sim 2 \text{ eV}$ ," J. Chem. Phys. 63, 3238-3242, 1975.

<sup>15</sup>F. C. Fehsenfeld, private communication, 1977.

<sup>16</sup>See for example, A. P. Mitra, "D-Region in Disturbed Condition, Including Flares and Energetic Particles," J. Atmos. and Terr. Phys. 37, 895-913, 1975.

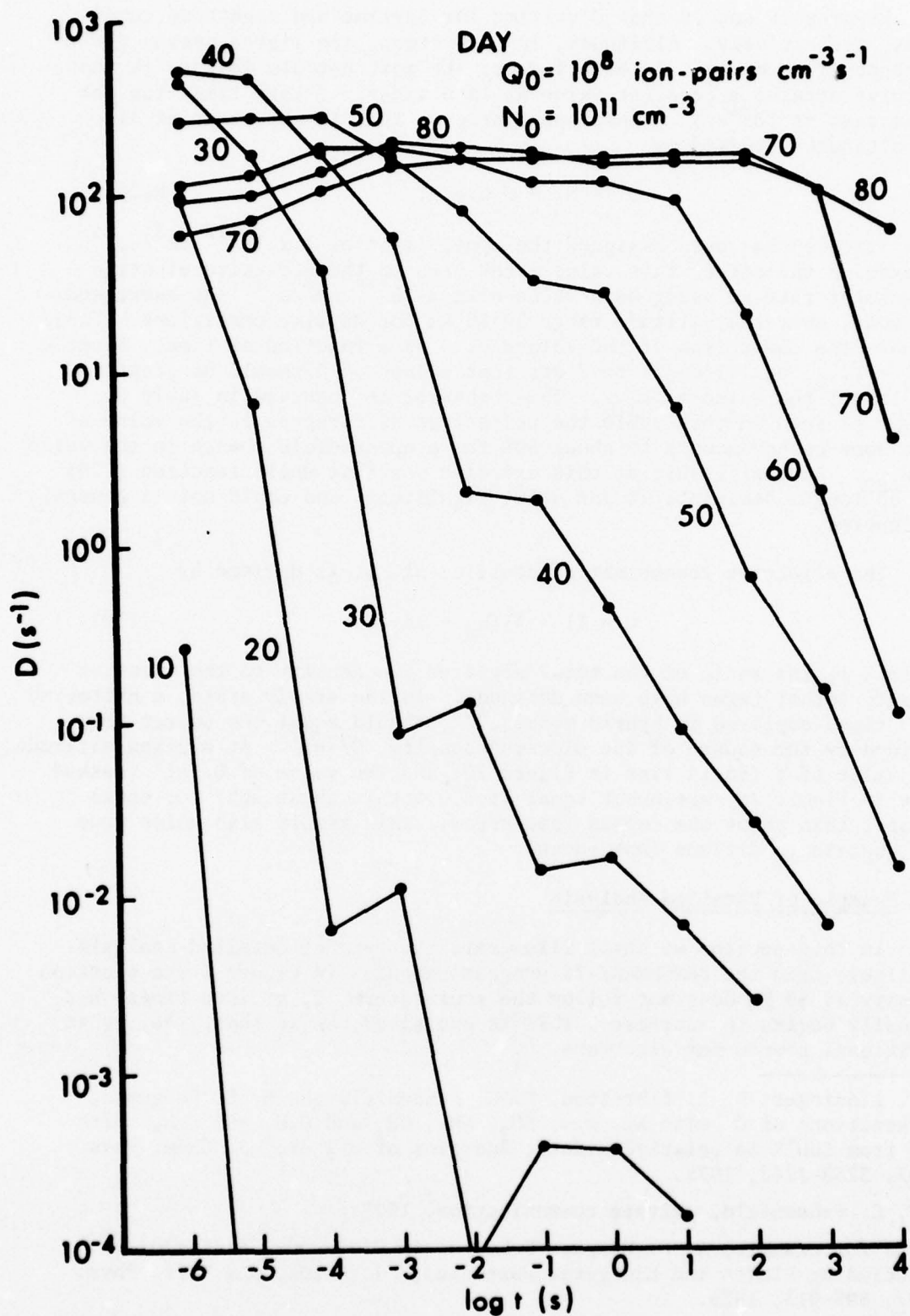


Figure 18. Effective electron detachment coefficient,  $D$ , as a function of time for daytime conditions. Parameters are the altitudes in km.

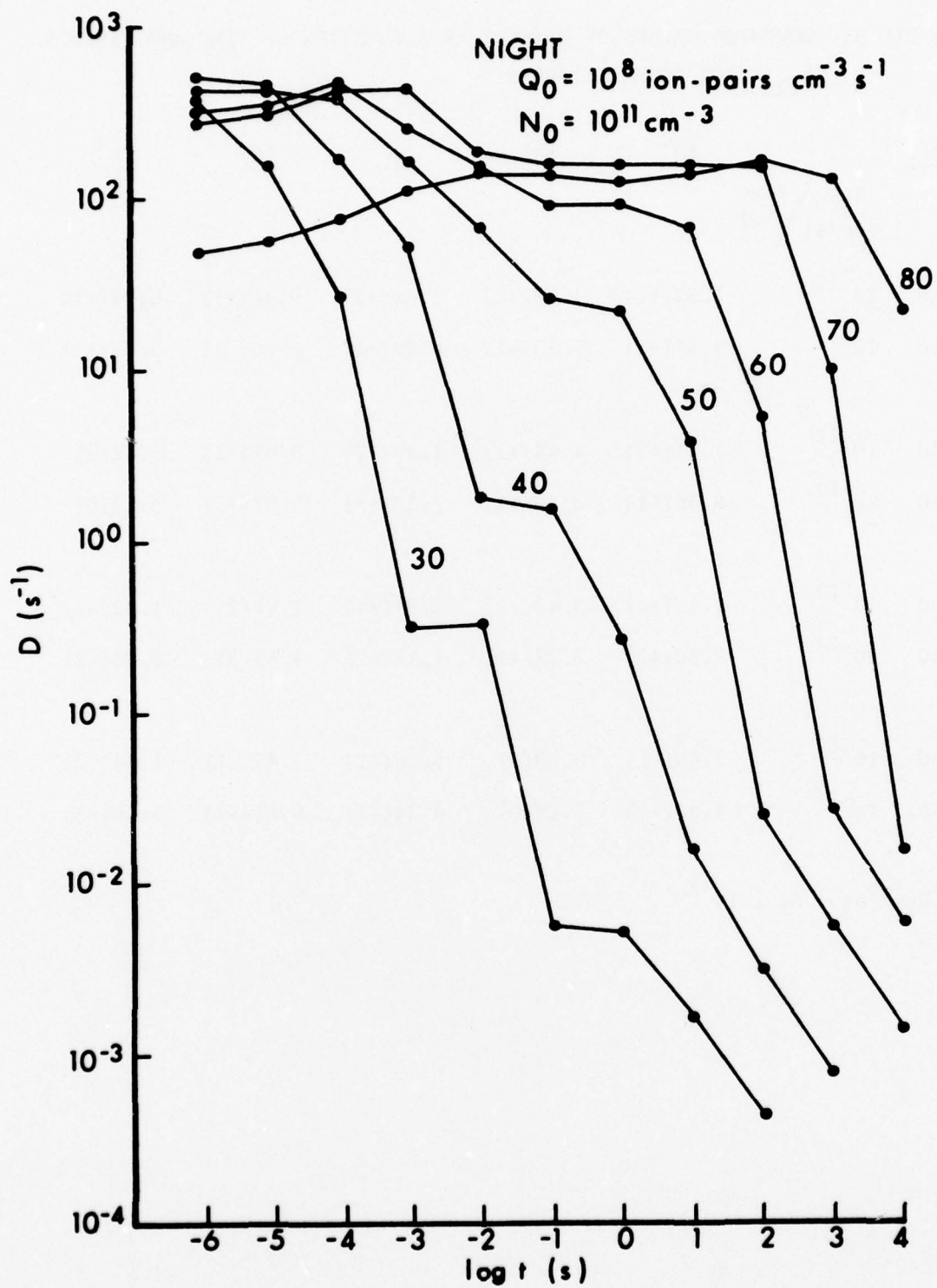


Figure 19. Same as Figure 18, except nighttime conditions.



TABLE 3. COMPUTED VALUES OF  $D$  ( $s^{-1}$ ) AS A FUNCTION OF TIME AND VALUE OF  $k_{129}$  FOR FOUR ALTITUDES.

ALT	$k_{129}$ / time (cc/s) / (s)	$10^0$	$10^1$	$10^2$	$10^3$	$10^4$
80	$10^{-12}$	1.32(+2)*	1.39(+2)	1.39(+2)	9.16(+1)	5.01(+1)
80	$10^{-14}$	9.57(+1)	9.53(+1)	8.89(+1)	6.56(+1)	3.85(+1)
70	$10^{-12}$	1.41(+2)	1.44(+2)	1.48(+2)	9.67(+1)	3.82(0)
70	$10^{-14}$	9.46(+1)	8.99(+1)	7.38(+1)	5.57(+1)	3.12(0)
60	$10^{-12}$	1.11(+2)	8.43(+1)	1.94(+1)	1.92(0)	1.02(-1)
60	$10^{-14}$	7.34(+1)	5.25(+1)	1.17(+1)	1.69(0)	9.23(-2)
50	$10^{-12}$	2.66(+1)	5.90(0)	6.06(-1)	1.43(-1)	1.34(-2)
50	$10^{-14}$	1.44(+1)	3.29(0)	4.24(-1)	9.61(-2)	5.56(-3)

\* Read as  $1.32 \times 10^{+2}$

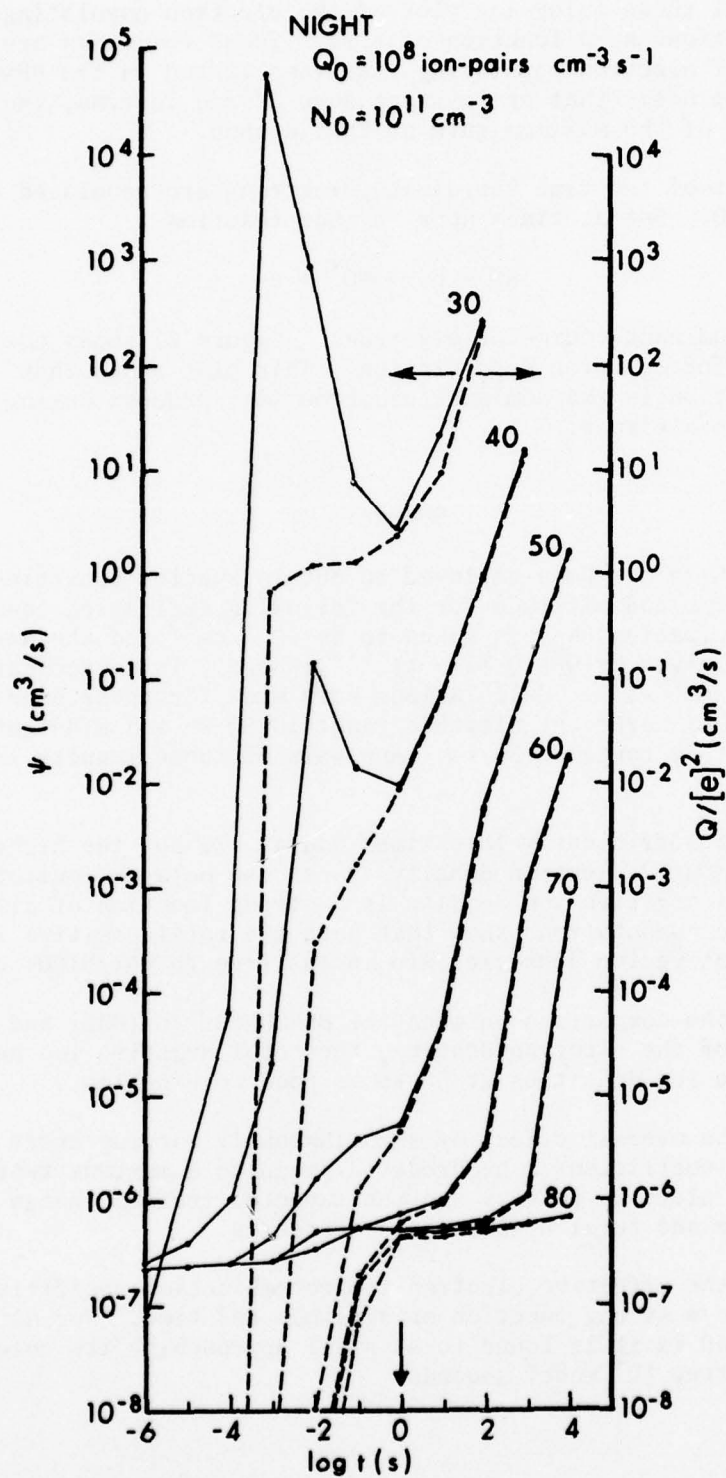
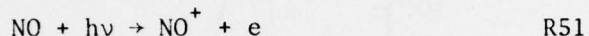


Figure 20. Composite plot of the logarithm of the total recombination coefficient,  $\psi$  (solid line), and of  $Q/[e]^2$  (dashed line) as a function of the logarithm of time for nighttime conditions. Parameters are the altitudes in km. The arrow points to decade after which  $\psi \approx Q/[e]^2$ .

Figure 21 shows a log-log plot of the electron populating rates for specific reactions as a function of time. These reactions are selected from a host of electron populating reactions listed in the BENCHMARK-76 output, on the basis that at least at some decade in time, the specific rate is  $\geq 10\%$  of the maximum rate at that decade.

Over most of the time coordinate, electrons are populated by the source term,  $Q$ . But at times near  $10^4$  the reaction



becomes the dominant source of electrons. Figure 22 shows the corresponding plot for electron depopulation. This plot shows that electron-ion recombination is the dominant electron loss process during all model times for this altitude.

#### SUMMARY

BENCHMARK-76 has been employed to obtain species densities as a function of time and altitude for the following excitation conditions. The prompt ionization,  $N_0$ , is taken to be  $10^{11} \text{ cm}^{-3}$  and the delayed ionization is given by  $Q = Q_0(1 + t)^{-1.2}$ , where  $t$  is in seconds and  $Q_0 = 10^5 \text{ ion pairs cm}^{-3}\text{-s}^{-1}$ . Calculations were made for three hour intervals around noon (DAY) over the altitude range 10-80 km and midnight (NIGHT) over the altitude range 30-80 km. Analysis of these results is summarized as follows.

First, at sufficiently late times and at all but the highest altitudes, the computed electron density tracks the delayed ionization. The computed total negative ion density is a strong function of altitude, as expected. The computations show that both the total positive ion and the total negative ion densities are insensitive to DAY/NIGHT conditions.

Second, the comparison between the BENCHMARK-76 (BRL) and DCHEM (MRC) computations of the electron density, the total negative ion and the total positive ion densities at 60 km is good to excellent.

Third, the overall effect of simultaneously varying every ion-ion recombination coefficient a hundredfold produced a maximum twofold change in the electron density and the expected tenfold change in both total positive and total negative ion densities.

Fourth, the effective electron-ion recombination coefficient,  $\alpha_d$ , is found to be a strong function of altitude and time. For altitudes greater than 40 km it is found to be still approaching its quiescent value, even after  $10^4$  model seconds.

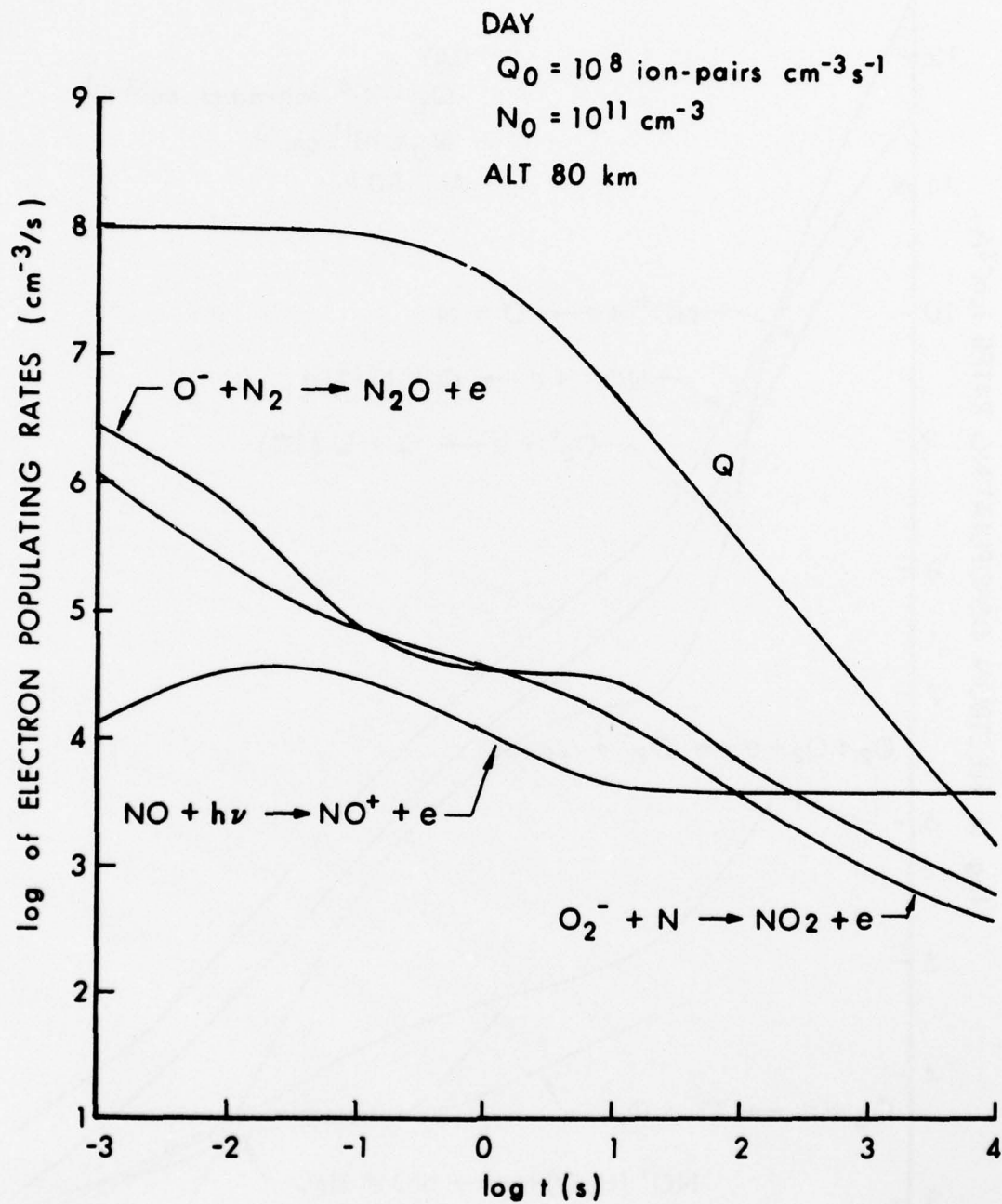


Figure 21. Logarithm of electron populating rates at 80 km vs. the logarithm of time for daytime conditions. Specific reactions are identified, Q is the delayed production of electrons.



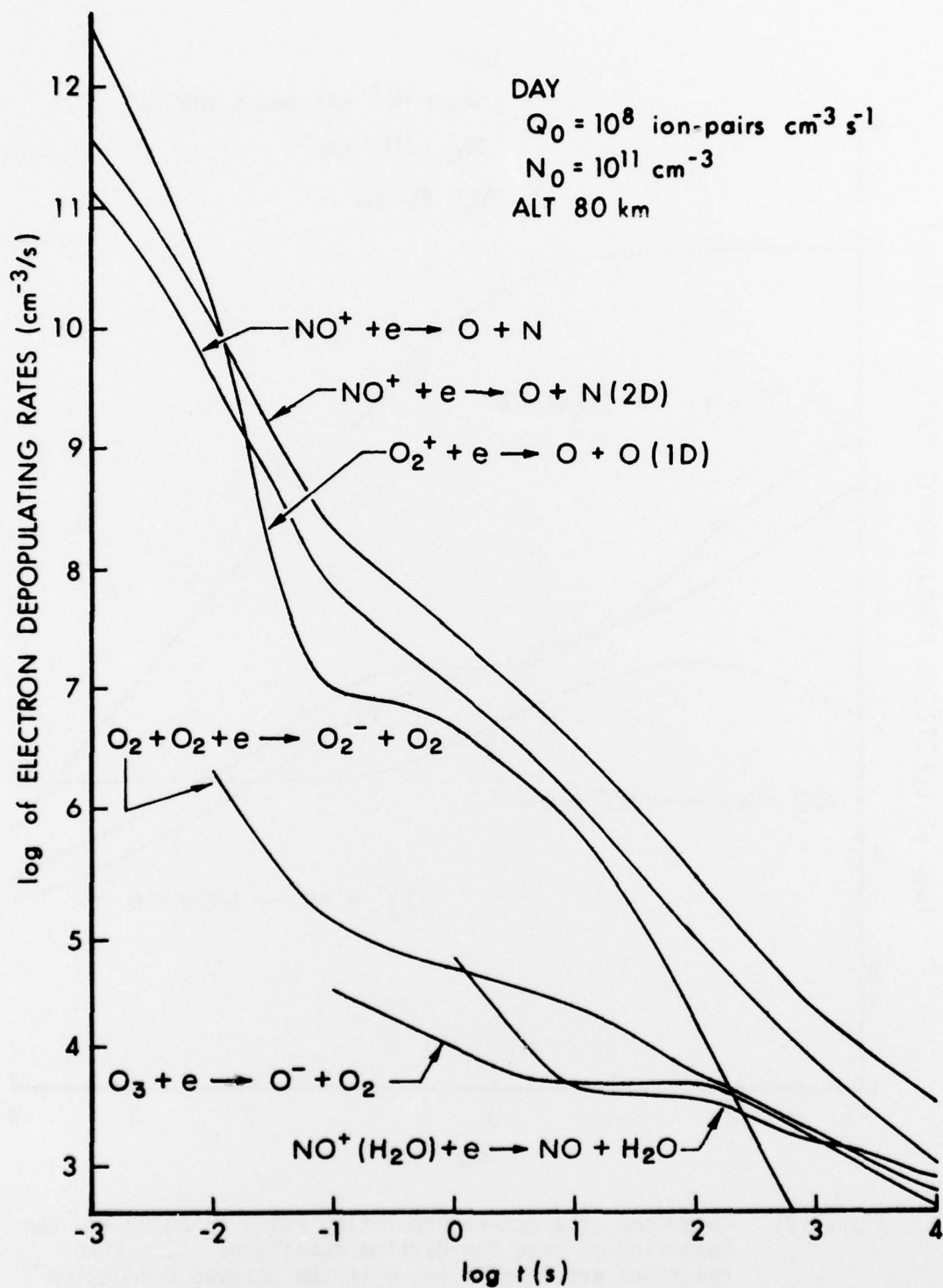


Figure 22. Logarithm of electron depopulating rates at 80 km vs. logarithm of time for daytime conditions. Specific reactions are identified.

Fifth, the effective electron attachment,  $A$ , is dominated by three body attachment to  $O_2$  and is not a function of time for altitudes below about 60 km. Increases of up to a factor of three in  $A$  at late times and at altitudes higher than 60 km are found to be caused by an increase in ozone which permits the reaction  $O_3 + e \rightarrow O^- + O_2$  to compete with  $O_2$  attachment.

Sixth, the effective electron detachment rate is found to be a strong function of time and altitude and under no conditions employed did it reach a constant value. The effective electron detachment rate is dominated by the reaction  $O^- + N_2 \rightarrow N_2O + e$  when a rate coefficient of  $1 \times 10^{-12}$  cm<sup>3</sup>/s is used. Even when this rate coefficient is reduced a hundredfold, the reaction in general can not be neglected.

Finally, the comparison of the effective recombination coefficient,  $\psi$ , and  $Q/[e]^2$  showed that a steady state is reached at all altitudes studied at about one second.

#### ACKNOWLEDGEMENT

To M. G. Heaps and G. E. Keller goes our thanks for reading an earlier version of this manuscript.

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2. F. Gilmore as quoted by B. F. Myers and M. R. Schoonover, "Electron Energy Degradation in the Atmosphere: Consequent Species and Energy Densities, Electron Flux, and Radiation Spectra," DNA 3513T, 3 Jan 75, Table 6.
3. J. M. Heimerl and F. E. Niles, "BENCHMARK-76: Model Computations for Disturbed Atmospheric Conditions I. Input Parameters," BRL Report No. 2022, October 1977. (AD #A050355)
4. F. E. Niles and J. M. Heimerl, "Selected Neutral Species Profiles 0-100 km," BRL Memo Report No. 2767, July 1977. (AD# A042620)
5. W. S. Knapp, "A Simplified D-Region Chemistry Model for Nuclear Environments," DNA-2850T, April 72; also M. Scheibe, Mission Research Corporation, private communication, 1976.
6. For example, The BENCHMARK-76 reaction set includes neutral odd-hydrogen reactions, while Scheibe's set does not.
7. J. M. Heimerl and F. E. Niles, "BENCHMARK-76: Model Computations for Disturbed Atmospheric Conditions III. Results for Selected Excitation Parameters at 60 km," BRL Technical Report ARBRL-TR-02051, March 1978.
8. D. Smith and M. J. Church, "Binary Ion-Ion Recombination Coefficients Determined in a Flowing Afterglow Plasma," Int. J. Mass Spec. and Ion. Phys. 19, 185, 1976.
9. For the case where selected  $\alpha_i$ 's are varied by the factors see "The Effects of Uncertainties in the Two-Body Ion-Ion Recombination Coefficient upon Computed Ion Distributions in the Stratosphere and Mesosphere," by J. M. Heimerl, BRL Report No. 1972, March 1977 (AD# A038263). Table 2 of this reference contains three typographical errors and one computational error. At 60 km the fourth reaction should read  $H^+(H_2O)_3 + NO_3^-$ ; at 40 km the third reaction  $H^+(H_2O)_4 + CO_3^-(H_2O)$  and at 30 km the first reaction  $H^+(H_2O)_4 + CO_3^-(H_2O)$ . The values in Table 3 of this reference then correspond to variations in the corrected ion-ion recombination reactions listed in Table 2. The computations at 40 km should have been carried out with  $H^+(H_2O)_4 + NO_3^-(H_2O)$  as the second reaction. Recomputation shows some changes in the percentages in Table 3 but the conclusions therein remain unchanged.
10. For a counter example wherein chemistry dominates the production term, see F. E. Niles, "Electron Density in the Beta Patch Following a Spartan Burst," BRL Report No. 1518, December 1970, Figure 9. (AD# 879464)

#### REFERENCES (CONTD)

11. Reactions 138-162 inclusive; see Appendix for reaction list.
12. Reactions 122-126 inclusive; see Appendix for reaction list.
13. Reactions 1-5 and 11 for photodetachment; 127-137 inclusive for two body collisional detachment; see Appendix for reaction list.
14. W. Lindinger, D. L. Albritton, F. C. Fehsenfeld and E. E. Ferguson, "Reactions of  $O^-$  with  $N_2$ ,  $N_2O$ ,  $SO_2$ ,  $NH_3$ ,  $CH_4$  and  $C_2H_4$  and  $C_2H_2^-$  with  $O$  from 300°K to relative kinetic energies of  $\sim 2$  eV," J. Chem. Phys. 63, 3238-3242, 1975.
15. F. C. Fehsenfeld, private communication, 1977.
16. See for example, A. P. Mitra, "D-Region in Disturbed Condition, Including Flares and Energetic Particles," J. Atmos. and Terr. Phys. 37, 895-913, 1975.



## APPENDIX

The table in this Appendix displays the nominal 496 reactions that link the 64 species within the BENCHMARK-76 code. Reactions proceed from left to right only. Each rate coefficient,  $k$ , is constructed from the reaction parameters  $A$ ,  $B$  and  $C$ , i.e.

$$k = A(T/300)^B \exp (- C/T) ,$$

where  $T$  is the temperature in degrees Kelvin. Except for the first 60 reactions, involving a photon as a reactant, the reference for the value of the rate coefficient is given to the right of the parameter  $C$  column. Further details can be obtained from Reference 3.

TABLE A. BENCHMARK-76 REACTION SET  
WAVELENGTH REGION

REAC. NO.	REACTION	REFERENCE	REF. NO.
1	N02- + HV = N02 + E		1
2	O- + HV = O + E		2
3	O- + HV = O1U + E		3
4	O2- + HV = O2 + E		4
5	O3- + HV = O3 + E		5
6	C03- + HV = C02 + O-		6
7	78- + HV = C03- + H2O		7
8	C04- + HV = O2- + C02		8
9	94- + HV = C04- + H2O		9
10	64- + HV = N02- + H2O		10
11	N03- + HV = O + N02 + E		11
12	62- + HV = N0 + O2-		12
13	80- + HV = N03- + H2O		13
14	125- + HV = N03- + H0O3		14
15	O2-W + HV = O2- + H2O		15
16	O3- + HV = O- + O2		16
17	O4- + HV = O2- + O2		17
18	N074 + HV = N0 + C02		18
19	N048 + HV = N0 + H2O		19
20	N058 + HV = N0 + V2		20
21	N092 + HV = N048 + C02		21
22	N066 + HV = H3O + HNO2		22
23	N066 + HV = N048 + H2O		23
24	N076 + HV = N048 + N2		24
25	N110 + HV = N066 + C02		25
26	N084 + HV = N066 + H2O		26
27	N094 + HV = N066 + N2		27
28	64+ + HV = N02+ + H2O		28
29	82+ + HV = 64+ + H2O		29
30	O250 + HV = O2+ + H2O		30
31	O260 + HV = O2+ + N2		31
32	O4+ + HV = O2+ + O2		32
33	H2 + HV = H + H		33
34	H2O + HV = H + H2O		34
35	H2O2 + HV = H2O + H2O		35
36	HNO2 + HV = H2O + N2		36
37	HNO3 + HV = H2O + N2		37
38	H2 + HV = H2 + J		38
39	N3 + HV = N + O		39
40	N02 + HV = N0 + O		40
41	N2 + HV = N2U + N		41
42	N2O + HV = N2 + O1U		42
43	O2 + HV = O + O		43
44	O2 + HV = O + O1U		44
45	O2 + HV = O21U		45
46	O2 + HV = O21S		46
47	O3 + HV = O + O2		47
48	O3 + HV = O + O21U		48
49	O3 + HV = O1U + O21U		49
50	N + HV = N+ + E		50
51	N0 + HV = N0+ + E		51
52	N02 + HV = N02+ + E		52
53	N2 + HV = N + N+ + E		53
54	N2 + HV = N2U + N+ + E		54
55	N2 + HV = N2+ + E		55
56	O + HV = O+ + E		56
57	O2 + HV = O2+ + E		57
58	O2 + HV = O + O+ + E		58
59	O2 + HV = O1U + O+ + E		59
60	O21U + HV = O2+ + E		60

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REF. NO.	REAC. NO.	REACTION	A	B	C	REFERENCE	REF. NO.
61	61	H + H2O2 = H2O + H2O	5.3E-10	0	4500	BAULCH ET AL HI TEMP REAC RATE DATA, LEEDS	61
62	62	H + H2O2 = H2 + H2O	2.8E-12	0	1900	HAMPSON+LD NBSIR-73-207 AUG 73	62
63	63	H + H2O = H2 + O	4.2E-12	1.0	3500	HAMPSON + GARVIN,ED NBS-TN-866	63
64	64	H + H2O2 = H2 + O2	4.2E-11	0	350	HAMPSON + GARVIN,ED NBS-TN-866	64
65	65	H + H2O2 = H2O + H2O	4.2E-11	0	950	HAMPSON + GARVIN,ED NBS-TN-866	65
66	66	H + H2O2 = H2O + O	8.3E-11	0	500	HAMPSON + GARVIN,ED NBS-TN-866	66
67	67	H + H2O2 = H2O + H2O	5.8E-10	0	740	HAMPSON + GARVIN,ED NBS-TN-866	67
68	68	H + H2O2 = H2 + H2O	1.3E-10	0	7600	HAMPSON + GARVIN,ED NBS-TN-866	68
69	69	H + H2O2 = O2 + O + H2O	3.7E-10	0	8450	HAMPSON + GARVIN,ED NBS-TN-866	69
70	70	H + H2O2 = H2O + O2	2.6E-11	0	0	HAMPSON + GARVIN,ED NBS-TN-866	70
71	71	H + H2O2 = H2 + H2O	3.6E-11	0	2590	HAMPSON + GARVIN,ED NBS-TN-866	71
72	72	H + H2O2 = H2O + H2O	1.7E-11	0	910	HAMPSON + GARVIN,ED NBS-TN-866	72
73	73	H + H2O2 = H2O2 + H2O	2.1E-12	0	0	HAMPSON + GARVIN,ED NBS-TN-866	73
74	74	H + H2O2 = H2O2 + H2O	1.3E-13	0	0	HAMPSON + GARVIN,ED NBS-TN-866	74
75	75	H + H2O2 = H2O2 + H2O	1.0E-11	0	550	HAMPSON + GARVIN,ED NBS-TN-866	75
76	76	H + H2O2 = H2O2 + H2O	6.0E-11	0	1000	HAMPSON + GARVIN,ED NBS-TN-866	76
77	77	H + H2O2 = H2O2 + H2O	1.6E-12	0	500	HAMPSON + GARVIN,ED NBS-TN-866	77
78	78	H + H2O2 = H2O2 + H2O	3.0E-11	0	1250	HAMPSON + GARVIN,ED NBS-TN-866	78
79	79	H + H2O2 = H2O2 + H2O	1.0E-13	0	0	HAMPSON + GARVIN,ED NBS-TN-866	79
80	80	H + H2O2 = H2O2 + H2O	5.3E-11	0	0	HAMPSON + GARVIN,ED NBS-TN-866	80
81	81	H + H2O2 = H2O2 + H2O	1.4E-11	0	0	HAMPSON + GARVIN,ED NBS-TN-866	81
82	82	H + H2O2 = H2O2 + H2O	1.4E-11	0	0	HAMPSON + GARVIN,ED NBS-TN-866	82
83	83	H + H2O2 = H2O2 + H2O	1.4E-12	0	0	HAMPSON + GARVIN,ED NBS-TN-866	83
84	84	H + H2O2 = H2O2 + H2O	3.3E-12	1.0	3150	HAMPSON + GARVIN,ED NBS-TN-866	84
85	85	H + H2O2 = H2O2 + H2O	5.7E-13	0	0	HAMPSON + GARVIN,ED NBS-TN-866	85
86	86	H + H2O2 = H2O2 + H2O	7.5E-12	0	0	SLANGER, WOOD + BLACK JGR 76, 8430 71	86
87	87	H + H2O2 = H2O2 + H2O	2.0E-13	0	1200	HAMPSON + GARVIN,ED NBS-TN-866	87
88	88	H + H2O2 = H2O2 + H2O	9.0E-13	0	2125	HAMPSON + GARVIN,ED NBS-TN-866	88
89	89	H + H2O2 = H2O2 + H2O	2.8E-12	0	0	HAMPSON + GARVIN,ED NBS-TN-866	89
90	90	H + H2O2 = H2O2 + H2O	4.2E-11	0	500	HAMPSON + GARVIN,ED NBS-TN-866	90
91	91	H + H2O2 = H2O2 + H2O	8.0E-11	0	0	HAMPSON + GARVIN,ED NBS-TN-866	91
92	92	H + H2O2 = H2O2 + H2O	9.1E-12	0	0	HAMPSON + GARVIN,ED NBS-TN-866	92
93	93	H + H2O2 = H2O2 + H2O	1.0E-11	0	2300	HAMPSON + GARVIN,ED NBS-TN-866	93
94	94	H + H2O2 = H2O2 + H2O	1.0E-11	0	2300	HAMPSON + GARVIN,ED NBS-TN-866	94
95	95	H + H2O2 = H2O2 + H2O	2.9E-10	0	0	HAMPSON + GARVIN,ED NBS-TN-866	95
96	96	H + H2O2 = H2O2 + H2O	3.5E-10	0	0	HAMPSON + GARVIN,ED NBS-TN-866	96
97	97	H + H2O2 = H2O2 + H2O	5.5E-11	0	0	HAMPSON + GARVIN,ED NBS-TN-866	97
98	98	H + H2O2 = H2O2 + H2O	1.1E-10	0	0	GARVIN,ED NBSIR 73-206	98
99	99	H + H2O2 = H2O2 + H2O	7.4E-11	0	0	HAMPSON + GARVIN,ED NBS-TN-866	99
100	100	H + H2O2 = H2O2 + H2O	2.5E-10	0	0	HAMPSON + GARVIN,ED NBS-TN-866	100
101	101	H + H2O2 = H2O2 + H2O	2.2E-18	0	0	HAMPSON + GARVIN,ED NBS-TN-866	101
102	102	H + H2O2 = H2O2 + H2O	2.0E-18	0	0	ARNOLD + OGRYZLO, CAN J PHYS 45, 2053 67	102
103	103	H + H2O2 = H2O2 + H2O	2.0E-15	0	0	HAMPSON + GARVIN,ED NBS-TN-866	103
104	104	H + H2O2 = H2O2 + H2O	2.5E-11	0	0	GILPIN, SCHIFF + WELGE, J CHEM PHYS 55, 1087 71	104
105	105	H + H2O2 = H2O2 + H2O	8.3E-33	0	0	HAMPSON + GARVIN,ED NBS-TN-866	105
106	106	H + H2O2 = H2O2 + H2O	6.8E-31	-2.0	0	HAMPSON + GARVIN,ED NBS-TN-866	106
107	107	H + H2O2 = H2O2 + H2O	2.0E-32	0	0	HAMPSON + GARVIN,ED NBS-TN-866	107
108	108	H + H2O2 = H2O2 + H2O	2.1E-32	0	-290	HAMPSON + GARVIN,ED NBS-TN-866	108
109	109	H + H2O2 = H2O2 + H2O	2.5E-33	0	-2550	HAMPSON + GARVIN,ED NBS-TN-866	109
110	110	H + H2O2 = H2O2 + H2O	2.2E-30	-2.5	0	HAMPSON + GARVIN,ED NBS-TN-866	110
111	111	H + H2O2 = H2O2 + H2O	1.0E-31	0	0	ESTIMATED	111
112	112	H + H2O2 = H2O2 + H2O	8.3E-34	0	-500	HAMPSON + GARVIN,ED NBS-TN-866	112
113	113	H + H2O2 = H2O2 + H2O	1.0E-32	-0.5	0	HAMPSON + GARVIN,ED NBS-TN-866	113
114	114	H + H2O2 = H2O2 + H2O	3.5E-33	0	-526	HAMPSON + GARVIN,ED NBS-TN-866	114
115	115	H + H2O2 = H2O2 + H2O	4.0E-33	0	-940	HAMPSON + GARVIN,ED NBS-TN-866	115
116	116	H + H2O2 = H2O2 + H2O	1.3E-32	-1.0	170	HAMPSON + GARVIN,ED NBS-TN-866	116
117	117	H + H2O2 = H2O2 + H2O	1.1E-34	0	-510	HAMPSON + GARVIN,ED NBS-TN-866	117
118	118	H + H2O2 = H2O2 + H2O	2.8E-36	0	0	HAMPSON + GARVIN,ED NBS-TN-866	118
119	119	H + H2O2 = H2O2 + H2O	6.8E-03	0	0	DNA HANDBOOK 1948H REV3 TABLE 24 REACTION XXX-1	119
120	120	H + H2O2 = H2O2 + H2O	2.6E-04	0	0	DNA HANDBOOK 1948H REV3 TABLE 24 REACTION XXX-5	120

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REAC. NO.	REACTION	A	B	C	REFERENCE	REF. NO.
121	021S = O2 + H2	8.3E-02	0	0	DNA HANDBOOK 1948H REV3 TABLE 24 REACTION XXX-6	121
122	022 + E = N2	4.0E-11	0	0	DNA HANDBOOK REV3 TABLE 24 REACTION IX-7 SAT 38	122
123	023 + E = O2 + H2	5.0E-08	0	0	FERGUSON ET AL DNA 3722E, AUG 75	123
124	03 + E = O2 + O2	9.0E-12	1.5	0	DNA HANDBOOK REV3 TABLE 24 REACTION IX-1 1 CHAN	124
125	02 + E = O2 + O2	1.4E-29	-1.0	600	DNA HANDBOOK REV3 TABLE 24 REACTION IX-2	125
126	02 + E = H2 + H2	1.0E-31	0	0	DNA HANDBOOK REV3 TABLE 24 REACTION IX-3	126
127	0 + E = H2 + H2	6.0E-10	-2	0	WCFARLAND ETAL J CHEM PHYS 59.6629 73	127
128	0 + E = N2 + N2	2.2E-10	0	0	DNA HANDBOOK	128
129	0 + E = N2 + N2	1.0E-12	0	0	LINDINGER ETAL J CHEM PHYS 63.3238.75 UP LIM	129
130	0 + E = N2 + N2	2.5E-10	-8	0	MCFARLAND ETAL J CHEM PHYS 59.6629 73	130
131	0 + E = O2 + E	2.0E-10	0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XII-1	131
132	0 + E = O2 + E	3.0E-10	0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XII-3	132
133	02 + E = N2 + O2 + E	3.0E-10	0	0	FEHSENFELD, PRIVATE COMMUNICATION	133
134	02 + E = N2 + O2 + E	1.9E-12	1.5	4990	DNA HANDBOOK REV3 TABLE 24 REACTION X-4	134
135	02 + E = O2 + E + O2	1.5E-10	0	0	F. C. FEHSENFELD, PRIVATE COMMUNICATION 75.	135
136	02 + E = O2 + E + O2	2.7E-10	5	5590	DNA HANDBOOK REV3 TABLE 24 REACTION X-5	136
137	02 + E = O2 + E + O2	2.0E-10	0	0	DNA HANDBOOK REV3 TABLE 24 REACTION X-6	137
138	030 + E = H + H2	1.5E-06	-2	0	DNA HANDBOOK REV4 TABLE 16-1	138
139	037 + E = H + H2	2.8E-06	-2	0	DNA HANDBOOK REV4 TABLE 16-1	139
140	036 + E = H + H2	3.0E-06	-1.0	0	DNA HANDBOOK	140
141	047 + E = H + H2	1.0E-06	-2	0	ESTIMATED	141
142	055 + E = H + H2	5.1E-06	-2	0	DNA HANDBOOK REV4 TABLE 16-1	142
143	073 + E = H + H2	6.1E-06	-2	0	DNA HANDBOOK REV4 TABLE 16-1	143
144	091 + E = H + H2	7.4E-06	-2	0	DNA HANDBOOK REV4 TABLE 16-1 KLEY ETAL JCP 66.4157.7	144
145	04 + E = O2 + N2	1.0E-07	-1.0	0	DNA HANDBOOK, EST.	145
146	04 + E = O2 + N2	3.0E-07	-1.0	0	DNA HANDBOOK, EST.	146
147	074 + E = N2 + CO2	1.0E-06	-2	0	DNA HANDBOOK, EST.	147
148	048 + E = N2 + CO2	1.0E-06	-2	0	DNA HANDBOOK, EST.	148
149	058 + E = N2 + CO2	1.0E-06	-2	0	DNA HANDBOOK, EST.	149
150	092 + E = N2 + CO2	1.0E-06	-2	0	DNA HANDBOOK, EST.	150
151	066 + E = N2 + CO2	2.0E-06	-2	0	DNA HANDBOOK, EST.	151
152	075 + E = N2 + CO2	1.0E-06	-2	0	DNA HANDBOOK, EST.	152
153	110 + E = N2 + H2 + H2	3.0E-06	-2	0	DNA HANDBOOK REV3 TABLE 24 REACTION IV-10	153
154	084 + E = N2 + H2 + H2	1.0E-06	-2	0	DNA HANDBOOK, EST.	154
155	094 + E = N2 + H2 + H2	3.0E-07	-5	0	DNA HANDBOOK, EST.	155
156	02 + E = N2 + H2	1.0E-06	-5	0	DNA HANDBOOK, EST.	156
157	64 + E = N2 + H2	2.0E-05	-5	0	DNA HANDBOOK, EST.	157
158	82 + E = N2 + H2	2.7E-07	-5	0	DNA HANDBOOK REV4 FIGURE 16-1 ESTIMATED PRODUCT	158
159	02 + E = O2 + H2	2.1E-07	-7	0	DNA HANDBOOK, TABLE 24-1.	159
160	0250 + E = O2 + H2	1.5E-06	-2	0	DNA HANDBOOK, EST.	160
161	04 + E = O2 + O2	2.0E-06	-1.0	0	DNA HANDBOOK, EST.	161
162	04 + E = O2 + O2	2.8E-10	0	0	DNA HANDBOOK REV3 TABLE 24 REACTION IV-11	162
163	02 + E = N2 + O2	5.0E-11	-8	0	WCFARLAND ETAL J C P 59.6620 73 T<4600.8/R=.5	163
164	02 + E = N2 + O2	2.9E-10	0	0	WCFARLAND ETAL J CHEM PHYS 59.6620 73 T<3560	164
165	04 + E = N2 + O2	1.0E-10	0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIII-27	165
166	82 + E = N2 + O2	1.0E-10	0	0	DNA HANDBOOK, EST.	166
167	02 + E = O2 + O2	1.0E-10	0	0	DNA HANDBOOK, EST.	167
168	02 + E = O2 + O2	2.0E-11	-4	0	MCFARLAND ETAL J CHEM PHYS 59.6620 73 T<1800	168
169	02 + E = O2 + O2	4.4E-10	0	0	LINDINGER ETAL JGR 80.3725 75	169
170	0250 + E = N2 + O2	6.6E-10	0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIII-16	170
171	0250 + E = N2 + O2	1.0E-10	0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-26 EST	171
172	0250 + E = N2 + O2	1.0E-10	0	0	ESTIMATED	172
173	04 + E = O2 + O2	5.0E-10	0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-23 EST	173
174	04 + E = O2 + O2	5.0E-10	0	0	ESTIMATED	174
175	030 + E = N2 + O2	1.6E-09	0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75	175
176	036 + E = N2 + O2	1.4E-09	0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-33	176
177	047 + E = N2 + O2	1.0E-09	0	0	ESTIMATED	177
178	074 + E = N2 + O2	2.4E-10	0	0	WCFARLAND ETAL J C P 59.6620.73 T<4600.8/R=.5	178
179	074 + E = N2 + O2	1.0E-09	0	0	ESTIMATED	179
180	048 + E = N2 + O2	5.0E-10	0	0	ESTIMATED, ANALOGY WITH 11048 + H2O2	180



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REAC. NO.	REACTION	A	B	C	REFERENCE	REF. NO.
181	N048 + H0 = H30+ + N02	6.0E-11	.0	0	FEHSENFELD + FERGUSON RAD SCI 7.113 72 UP-LIM	181
182	N048 + H202 = H30+ + N02 + H0	3.0E-11	.0	0	ESTIMATED	182
183	N048 + H202 = N02+ + H20 + H20	3.0E-11	.0	0	ESTIMATED	183
184	N048 + H202 = 64+ + H20	3.0E-11	.0	0	ESTIMATED	184
185	N058 + H20 = N074 + N2	1.0E-09	.0	0	ESTIMATED	185
186	N058 + H20 = N048 + N2	1.0E-09	.0	0	ESTIMATED	186
187	N092 + H20 = N066 + C02	1.0E-09	.0	0	ESTIMATED	187
188	N076 + C02 = N092 + N2	1.0E-09	.0	0	ESTIMATED	188
189	N110 + H20 = N084 + C02	1.0E-09	.0	0	ESTIMATED	189
190	N084 + H20 = H+55 + HNU2	7.0E-11	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-30	190
191	N094 + C02 = N110 + N2	1.0E-09	.0	0	ESTIMATED	191
192	64+ + N0 = N048 + N02	3.1E-11	.0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75	192
193	82+ + H20 = H+37 + HNO3	1.0E-11	.0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75 LOW LIM	193
194	N2+ + O = N20 + N	1.0E-11	.0	0	MCFARLAND ETAL JGR 79.2925 74 B/R EST.	194
195	N2+ + O = N20 + N	1.5E-10	-2	0	MCFARLAND ETAL JGR 79.2925 74 B/R EST.	195
196	N2+ + O = N20 + N	1.2E-12	-1.0	0	MCFARLAND ETAL J CHEM PHYS 59.6620 73 T<750	196
197	O+ + N2 = N0+ + N	1.6E-10	.0	0	DNA HANDBOOK TABLE 24	197
198	O2+ + N2 = N0+ + N0	1.0E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-9 EST	198
199	O250 + H20 = H30+ + H0 + O2	2.0E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-27A	199
200	O250 + H20 = H+36 + O2	1.0E-09	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-27B	200
201	O250 + O2 = O4+ + N2	2.0E-10	.0	2300	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-25 EST	201
202	O260 + O2 = O4+ + N2	1.0E-09	.0	0	ESTIMATED	202
203	O4+ + O = O2+ + O3	1.5E-09	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-24	203
204	H30+ + H20 = H+37 + M	3.0E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-22	204
205	H30+ + H20 + M = H+37 + M	3.4E-27	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIV-13B	205
206	H30+ + H20 + M = H+47 + M	1.4E-30	-2.0	0	ESTIMATED	206
207	H+37 + H20 + M = H+55 + M	2.3E-27	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-14B	207
208	H+55 + H20 + M = H+73 + M	2.4E-27	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-15B	208
209	H+73 + H20 + M = H+91 + M	9.0E-28	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-16	209
210	N0+ + C02 + M = V074 + M	2.4E-29	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-10B	210
211	N0+ + H20 + M = N048 + M	1.5E-28	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-9	211
212	N0+ + N2 + M = N058 + M	2.0E-31	-4.4	0	JOHNSON ETAL J CHEM PHYS 63.5374 75	212
213	N048 + C02 + M = N092 + M	2.0E-29	-2.0	0	ESTIMATED	213
214	N048 + H20 + M = N066 + M	1.1E-27	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-11	214
215	N048 + N2 + M = N076 + M	2.0E-31	-4.4	0	ESTIMATED	215
216	N066 + C02 + M = N110 + M	2.0E-29	-2.0	0	ESTIMATED	216
217	N066 + H20 + M = N084 + M	1.6E-27	-2.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XIX-12	217
218	N066 + N2 + M = N094 + M	2.0E-31	-4.4	0	ESTIMATED	218
219	N02+ + H20 + M = 64+ + M	5.0E-28	-2.0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75 TEMP EST	219
220	64+ + H20 + M = 82+ + M	2.0E-27	-2.0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75 TEMP EST	220
221	O+ + N2 + M = N0+ + N + M	6.0E-29	-2.0	0	DNA HANDBOOK TABLE 18A-5 TAKE (17/82)**-2.X3.8	221
222	O2+ + H20 + M = O250 + M	2.8E-28	-2.0	0	FEHSENFELD ETAL J CHEM PHYS 55.2115 71 MEN2	222
223	O2+ + O2 + M = O4+ + N	3.9E-30	-3.2	0	PAYZANT ETAL J CHEM PHYS 59.5615 73 XI.5	223
224	O2+ + N2 + M = O260 + M	9.0E-31	-2.0	0	DNA HANDBOOK TABLE 18A-5 TAKE (17/200)**-2.X3.8	224
225	H+36 + M = H30+ + H0 + M	3.0E-31	-2.0	12000	ESTIMATED	225
226	H+37 + M = H30+ + H20 + M	1.6E-01	-2.0	18200	ESTIMATED	226
227	H+47 + M = H30+ + N2 + M	1.1E-08	-2.0	1900	ESTIMATED	227
228	H+55 + M = H+37 + H20 + M	1.6E-01	-2.0	11300	ESTIMATED	228
229	H+73 + M = H+55 + H20 + M	1.0E-01	-2.0	8600	ESTIMATED	229
230	H+91 + M = H+73 + H20 + M	1.3E-00	-2.0	7700	ESTIMATED	230
231	N074 + M = N0+ + C02 + M	7.8E-09	-2.0	5600	ESTIMATED	231
232	N058 + M = N0+ + N2 + M	1.1E-08	-4.4	1900	J CHEM PHY 60. 4362. 74 + JCP 63. 3374. 75	232
233	N092 + M = N048 + C02 + M	4.0E-09	-2.0	5600	ESTIMATED	233
234	N066 + M = N048 + H20 + M	5.9E-02	-2.0	8700	ESTIMATED	234
235	N076 + M = N048 + N2 + M	1.1E-08	-4.4	1900	ESTIMATED	235
236	N110 + M = N066 + C02 + M	4.0E-09	-2.0	5600	ESTIMATED	236
237	N084 + M = N066 + H20 + M	2.2E-02	-2.0	7000	ESTIMATED	237
238	N094 + M = N066 + N2 + M	1.1E-0A	-4.4	1900	ESTIMATED	238
239	O250 + O210 = O2+ + O2 + H20	1.0E-10	.0	0	ESTIMATED	239
240	O4+ + M = O2+ + O2 + M	1.2E-05	-3.2	5300	PAYZANT ETAL J CHEM PHYS 59. 5615. 73	240

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REAC. NO.	REACTION	A	B	C	REFERENCE	REF. NO.
241	CO <sub>2</sub> + O <sub>3</sub> = O <sub>3</sub> + CO <sub>2</sub> + O <sub>2</sub>	1.3E-10	.0	0	FEHSENFELD + FERGUSON J CHEM PHYS 61.3181 74	241
242	O <sub>2</sub> + NO <sub>2</sub> = O + NO <sub>2</sub>	1.2E-09	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XV-2	242
243	O <sub>2</sub> + O <sub>3</sub> = O + O <sub>3</sub>	5.3E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XV-3	243
244	O <sub>2</sub> + NO <sub>2</sub> = O <sub>2</sub> + NO <sub>2</sub>	1.2E-09	.0	0	FEHSENFELD + FERGUSON J CHEM PHYS 61.3181 74	244
245	O <sub>2</sub> + O <sub>2</sub> = O <sub>2</sub> + O <sub>2</sub>	1.5E-10	.0	0	F. C. FEHSENFELD, PRIVATE COMMUNICATION 75.	245
246	O <sub>2</sub> + O <sub>3</sub> = O <sub>2</sub> + O <sub>3</sub>	4.0E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XV-5	246
247	O <sub>2</sub> + O <sub>3</sub> = O <sub>2</sub> + O <sub>3</sub>	2.3E-10	.0	0	FEHSENFELD + FERGUSON J CHEM PHYS 61.3181 74	247
248	O <sub>2</sub> + O <sub>3</sub> = O <sub>2</sub> + O <sub>3</sub>	5.0E-10	.0	0	ESTIMATED	248
249	CO <sub>2</sub> + HNO <sub>3</sub> = NO <sub>3</sub> + H <sub>2</sub> O + CO <sub>2</sub>	4.0E-10	.0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75	249
250	CO <sub>2</sub> + NO <sub>2</sub> = NO <sub>2</sub> + CO <sub>2</sub>	9.0E-12	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-23	250
251	CO <sub>2</sub> + NO <sub>2</sub> = NO <sub>2</sub> + CO <sub>2</sub>	2.0E-11	.0	0	FEHSENFELD + FERGUSON J CHEM PHYS 61.3181 74	251
252	CO <sub>2</sub> + O <sub>2</sub> = O <sub>2</sub> + CO <sub>2</sub>	8.0E-11	.0	0	DNA HANDBOOK TABLE 24	252
253	CO <sub>2</sub> + NO <sub>2</sub> = NO <sub>2</sub> + CO <sub>2</sub>	7.0E-12	.0	0	FEHSENFELD + FERGUSON J CHEM PHYS 61.3181 74	253
254	CO <sub>2</sub> + NO <sub>2</sub> = NO <sub>2</sub> + CO <sub>2</sub>	4.8E-11	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-27	254
255	CO <sub>2</sub> + NO <sub>2</sub> = NO <sub>2</sub> + CO <sub>2</sub>	1.5E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-25	255
256	CO <sub>2</sub> + NO <sub>2</sub> = NO <sub>2</sub> + CO <sub>2</sub>	4.3E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-26 EST	256
257	CO <sub>2</sub> + NO <sub>2</sub> = NO <sub>2</sub> + CO <sub>2</sub>	5.0E-10	.0	0	ESTIMATED	257
258	CO <sub>2</sub> + NO <sub>2</sub> = NO <sub>2</sub> + CO <sub>2</sub>	1.6E-09	.0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75	258
259	CO <sub>2</sub> + NO <sub>2</sub> = NO <sub>2</sub> + CO <sub>2</sub>	2.0E-13	.0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75 UP LIM	259
260	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	1.8E-11	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-10	260
261	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	5.0E-10	.0	0	ESTIMATED	261
262	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	1.5E-11	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-15	262
263	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	5.0E-10	.0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75 LOW LIM	263
264	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	3.0E-09	.0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75	264
265	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.8E-09	.0	0	FEHSENFELD ETAL J CHEM PHYS 63.2835 75	265
266	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	1.0E-10	.0	0	FEHSENFELD, PRIVATE COMMUNICATION	266
267	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	5.8E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-21	267
268	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	3.1E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-20	268
269	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	5.5E-10	.0	0	FEHSENFELD + FERGUSON J CHEM PHYS 61.3181 74	269
270	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.8E-12	.0	0	F. C. FEHSENFELD, PRIVATE COMMUNICATION 75.	270
271	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.8E-10	.0	0	DUNKIN ETAL CHEM PHYS LET 15.257 72	271
272	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	3.2E-10	.0	0	F. C. FEHSENFELD, PRIVATE COMMUNICATION 75.	272
273	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	4.3E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-19	273
274	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	1.4E-09	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-18	274
275	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.5E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-17	275
276	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	4.0E-10	.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XVI-16	276
277	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	1.0E-28	-1.0	0	J CHEM PHYS 61.3181 74 M=02 TEMP DEP ESTIMATED	277
278	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	5.0E-29	-1.0	0	ESTIMATED	278
279	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	1.3E-28	-1.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XXIII-11	279
280	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	7.5E-29	-1.0	0	PAYZANT, PRIVATE COMMUNICATION 72	280
281	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	3.1E-28	-1.0	0	J CHEM PHYS 61.3181 74 M=02 TEMP DEP ESTIMATED	281
282	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	1.1E-30	-1.0	0	PARKES, TRAN FAR SOC 67.711 71 M=02 TEMP DEP EST	282
283	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-29	-1.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XXIII-9	283
284	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	3.0E-28	-1.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XXIII-8	284
285	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	3.5E-31	-1.0	0	DNA HANDBOOK REV3 TABLE 24 REACTION XXIII-6	285
286	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-05	-1.0	6300	DNA HANDBOOK REV3 TABLE 24 REACTION XXIV-1	286
287	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-07	-5	0	ESTIMATED	287
288	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-07	-5	0	ESTIMATED	288
289	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-07	-5	0	ESTIMATED	289
290	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-07	-5	0	ESTIMATED	290
291	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-07	-5	0	ESTIMATED	291
292	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-07	-5	0	ESTIMATED	292
293	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-07	-5	0	ESTIMATED	293
294	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-07	-5	0	ESTIMATED	294
295	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-07	-5	0	ESTIMATED	295
296	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-07	-5	0	ESTIMATED	296
297	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-07	-5	0	ESTIMATED	297
298	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-07	-5	0	ESTIMATED	298
299	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-07	-5	0	ESTIMATED	299
300	NO <sub>2</sub> + O <sub>3</sub> = NO <sub>3</sub> + O <sub>2</sub>	2.0E-07	-5	0	ESTIMATED	300

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REAC. NO.	REACTION	A	B	C	REFERENCE	REF. NO.
301	H3O+ + O4- = H2O + H2O + O2	2.0E-07	-5	0	ESTIMATED	301
302	H+37 + CO3- = H2O + CO2 + H2O	2.0E-07	-5	0	ESTIMATED	302
303	H+37 + 78- = CO2 + O + H2O + H2O + H	2.0E-07	-5	0	ESTIMATED	303
304	H+37 + CO4- = H2O + H2O + H2O + CO2	2.0E-07	-5	0	ESTIMATED	304
305	H+37 + 94- = CO2 + O2 + H2O + H2O + H	2.0E-07	-5	0	ESTIMATED	305
306	H+37 + NO2- = H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	306
307	H+37 + 64- = H + H2O + NO2 + H2O	2.0E-07	-5	0	ESTIMATED	307
308	H+37 + NO3- = H2O + H2O + H2O + NO2	2.0E-07	-5	0	ESTIMATED	308
309	H+37 + 62- = H2O + H2O + H2O + NO	2.0E-07	-5	0	ESTIMATED	309
310	H+37 + 80- = NO2 + H2O + H + H2O + H2O + O	2.0E-07	-5	0	ESTIMATED	310
311	H+37 + 125- = HNO3 + HNO3 + H2O + H2O	2.0E-07	-5	0	ESTIMATED	311
312	H+37 + O- = H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	312
313	H+37 + O2- = H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	313
314	H+37 + O2- = H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	314
315	H+37 + O3- = H2O + H2O + H2O + O2	2.0E-07	-5	0	ESTIMATED	315
316	H+37 + O4- = H2O + H2O + H2O + O2	2.0E-07	-5	0	ESTIMATED	316
317	H+55 + CO3- = H2O + H2O + CO2 + H2O + H2O	2.0E-07	-5	0	ESTIMATED	317
318	H+55 + 78- = CO2 + O + H2O + H2O + H2O + H	2.0E-07	-5	0	ESTIMATED	318
319	H+55 + CO4- = H2O + H2O + H2O + CO2	2.0E-07	-5	0	ESTIMATED	319
320	H+55 + 94- = CO2 + O2 + H2O + H2O + H2O + H	2.0E-07	-5	0	ESTIMATED	320
321	H+55 + NO2- = H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	321
322	H+55 + 64- = H + H2O + NO2 + H2O + H2O	2.0E-07	-5	0	ESTIMATED	322
323	H+55 + NO3- = H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	323
324	H+55 + 62- = H2O + H2O + H2O + NO	2.0E-07	-5	0	ESTIMATED	324
325	H+55 + 80- = NO2 + H2O + H + H2O + H2O + H2O + O	2.0E-07	-5	0	ESTIMATED	325
326	H+55 + 125- = HNO3 + HNO3 + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	326
327	H+55 + O- = H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	327
328	H+55 + O2- = H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	328
329	H+55 + O3- = H2O + H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	329
330	H+55 + O4- = H2O + H2O + H2O + H2O + O2	2.0E-07	-5	0	ESTIMATED	330
331	H+73 + CO3- = H2O + H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	331
332	H+73 + CO3- = H2O + H2O + H2O + CO2 + H2O	2.0E-07	-5	0	ESTIMATED	332
333	H+73 + 78- = H + H2O + H2O + H2O + H2O + CO2 + O + H2O	2.0E-07	-5	0	ESTIMATED	333
334	H+73 + CO4- = H2O + H2O + H2O + H2O + CO2 + H2O	2.0E-07	-5	0	ESTIMATED	334
335	H+73 + 94- = H + H2O + H2O + H2O + CO2 + O2 + H2O	2.0E-07	-5	0	ESTIMATED	335
336	H+73 + NO2- = H2O + H2O + H2O + H2O + H2O + NO	2.0E-07	-5	0	ESTIMATED	336
337	H+73 + 64- = H + H2O + H2O + H2O + H2O + NO2 + H2O	2.0E-07	-5	0	ESTIMATED	337
338	H+73 + NO3- = H2O + H2O + H2O + H2O + H2O + NO2	2.0E-07	-5	0	ESTIMATED	338
339	H+73 + 62- = H2O + H2O + H2O + H2O + H2O + NO	2.0E-07	-5	0	ESTIMATED	339
340	H+73 + 80- = H + H2O + H2O + H2O + H2O + NO2 + O + H2O	2.0E-07	-5	0	ESTIMATED	340
341	H+73 + 125- = HNO3 + HNO3 + H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	341
342	H+73 + O- = H2O + H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	342
343	H+73 + O2- = H2O + H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	343
344	H+73 + O3- = H2O + H2O + H2O + H2O + H2O + O2	2.0E-07	-5	0	ESTIMATED	344
345	H+73 + O4- = H2O + H2O + H2O + H2O + H2O + O2	2.0E-07	-5	0	ESTIMATED	345
346	H+91 + CO3- = H2O + H2O + H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	346
347	H+91 + CO3- = H2O + H2O + H2O + H2O + H2O + H2O + CO2	2.0E-07	-5	0	ESTIMATED	347
348	H+91 + 78- = H + H2O + H2O + H2O + H2O + H2O + CO2 + O + H2O	2.0E-07	-5	0	ESTIMATED	348
349	H+91 + CO4- = H2O + H2O + H2O + H2O + H2O + H2O + CO2 + H2O	2.0E-07	-5	0	ESTIMATED	349
350	H+91 + 94- = H + H2O + H2O + H2O + H2O + H2O + CO2 + O2 + H2O	2.0E-07	-5	0	ESTIMATED	350
351	H+91 + NO2- = H2O + H2O + H2O + H2O + H2O + H2O + NO	2.0E-07	-5	0	ESTIMATED	351
352	H+91 + 64- = H + H2O + H2O + H2O + H2O + H2O + NO2 + H2O	2.0E-07	-5	0	ESTIMATED	352
353	H+91 + NO3- = H2O + H2O + H2O + H2O + H2O + H2O + NO	2.0E-07	-5	0	ESTIMATED	353
354	H+91 + 62- = H2O + H2O + H2O + H2O + H2O + H2O + NO	2.0E-07	-5	0	ESTIMATED	354
355	H+91 + 80- = H + H2O + H2O + H2O + H2O + H2O + NO2 + O + H2O	2.0E-07	-5	0	ESTIMATED	355
356	H+91 + 125- = HNO3 + HNO3 + H2O + H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	356
357	H+91 + O- = H2O + H2O + H2O + H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	357
358	H+91 + O2- = H2O + H2O + H2O + H2O + H2O + H2O + H2O	2.0E-07	-5	0	ESTIMATED	358
359	H+91 + O3- = H2O + H2O + H2O + H2O + H2O + H2O + H2O + O2 + H2O	2.0E-07	-5	0	ESTIMATED	359
360	H+91 + O4- = H2O + H2O + H2O + H2O + H2O + H2O + H2O + O2 + H2O	2.0E-07	-5	0	ESTIMATED	360



[illegible]



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REF. NO.	REAC. NO.	REACTION	A	B	C	REFERENCE
421	421	$NO_8 + O_4 = O_2 + NO + H_2O + O_2 + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
422	422	$NO_2 + CO_3 = NO + O_2 + CO_2$	2.0E-07	-5	0	ESTIMATED
423	423	$NO_2 + NO = CO_2 + O_2 + H_2O + NO$	2.0E-07	-5	0	ESTIMATED
424	424	$NO_2 + NO_2 = CO_2 + O_2 + NO_2$	2.0E-07	-5	0	ESTIMATED
425	425	$NO_2 + NO_2 = CO_2 + O_2 + H_2O + NO + O$	2.0E-07	-5	0	ESTIMATED
426	426	$NO_2 + NO_2 = NO_2 + H_2O$	2.0E-07	-5	0	ESTIMATED
427	427	$NO_2 + NO_2 = NO_2 + H_2O + NO_2$	2.0E-07	-5	0	ESTIMATED
428	428	$NO_2 + NO_2 = NO_2 + NO_2 + O$	2.0E-07	-5	0	ESTIMATED
429	429	$NO_2 + NO_2 = NO_2 + NO_2 + NO$	2.0E-07	-5	0	ESTIMATED
430	430	$NO_2 + NO_2 = NO_2 + H_2O + NO + O_2$	2.0E-07	-5	0	ESTIMATED
431	431	$NO_2 + NO_2 = HNO_3 + NO_2 + NO + O_2$	2.0E-07	-5	0	ESTIMATED
432	432	$NO_2 + NO_2 = O_2 + NO$	2.0E-07	-5	0	ESTIMATED
433	433	$NO_2 + NO_2 = O_2 + NO + O$	2.0E-07	-5	0	ESTIMATED
434	434	$NO_2 + NO_2 = O_2 + H_2O + NO + O$	2.0E-07	-5	0	ESTIMATED
435	435	$NO_2 + NO_2 = O_2 + O_2 + NO$	2.0E-07	-5	0	ESTIMATED
436	436	$NO_2 + NO_2 = O_2 + O_2 + NO + O$	2.0E-07	-5	0	ESTIMATED
437	437	$NO_2 + NO_2 = O_2 + H_2O + CO_2 + O_2$	2.0E-07	-5	0	ESTIMATED
438	438	$NO_2 + NO_2 = NO + CO_2 + O_2 + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
439	439	$NO_2 + NO_2 = NO_2 + H_2O + CO_2 + O_2$	2.0E-07	-5	0	ESTIMATED
440	440	$NO_2 + NO_2 = NO_2 + H_2O + CO_2 + O_2 + H_2O$	2.0E-07	-5	0	ESTIMATED
441	441	$NO_2 + NO_2 = NO + NO + O_2 + H_2O$	2.0E-07	-5	0	ESTIMATED
442	442	$NO_2 + NO_2 = NO + NO + O_2 + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
443	443	$NO_2 + NO_2 = NO_2 + NO + O_2 + H_2O$	2.0E-07	-5	0	ESTIMATED
444	444	$NO_2 + NO_2 = NO_2 + NO + O_2 + H_2O$	2.0E-07	-5	0	ESTIMATED
445	445	$NO_2 + NO_2 = NO_2 + NO + O_2 + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
446	446	$NO_2 + NO_2 = NO_2 + NO + O_2 + H_2O + HNO_3$	2.0E-07	-5	0	ESTIMATED
447	447	$NO_2 + NO_2 = NO + O_2 + H_2O$	2.0E-07	-5	0	ESTIMATED
448	448	$NO_2 + NO_2 = NO + O_2 + H_2O$	2.0E-07	-5	0	ESTIMATED
449	449	$NO_2 + NO_2 = NO + O_2 + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
450	450	$NO_2 + NO_2 = NO + O_2 + O_2 + H_2O$	2.0E-07	-5	0	ESTIMATED
451	451	$NO_2 + NO_2 = NO + O_2 + O_2 + H_2O$	2.0E-07	-5	0	ESTIMATED
452	452	$NO_2 + NO_2 = NO + H_2O + CO_2 + O_2 + H_2O$	2.0E-07	-5	0	ESTIMATED
453	453	$NO_2 + NO_2 = NO + CO_2 + O_2 + H_2O + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
454	454	$NO_2 + NO_2 = NO_2 + H_2O + CO_2 + O_2 + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
455	455	$NO_2 + NO_2 = NO_2 + H_2O + CO_2 + O_2 + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
456	456	$NO_2 + NO_2 = NO + NO + O_2 + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
457	457	$NO_2 + NO_2 = NO + NO + O_2 + H_2O + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
458	458	$NO_2 + NO_2 = NO_2 + NO + O_2 + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
459	459	$NO_2 + NO_2 = NO_2 + NO + O_2 + H_2O + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
460	460	$NO_2 + NO_2 = NO_2 + NO + O_2 + H_2O + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
461	461	$NO_2 + NO_2 = NO_2 + NO + O_2 + H_2O + HNO_3 + H_2O$	2.0E-07	-5	0	ESTIMATED
462	462	$NO_2 + NO_2 = NO + O_2 + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
463	463	$NO_2 + NO_2 = NO + O_2 + H_2O + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
464	464	$NO_2 + NO_2 = NO + O_2 + O_2 + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
465	465	$NO_2 + NO_2 = NO + O_2 + O_2 + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
466	466	$NO_2 + NO_2 = NO + O_2 + O_2 + H_2O + H_2O$	2.0E-07	-5	0	ESTIMATED
467	467	$NO_2 + NO_2 = NO_2 + O_2 + H_2O + O_2$	2.0E-07	-5	0	ESTIMATED

REF. NO.	REACTION	A	B	C	REFERENCE
481	$02 + 04 = 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
482	$0250 + 03 = 02 + 02 + 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
483	$0250 + 78 = 02 + 02 + 02 + 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
484	$0250 + 04 = 02 + 02 + 02 + 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
485	$0250 + 94 = 02 + 02 + 02 + 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
486	$0250 + 02 = 02 + 02 + 02 + 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
487	$0250 + 64 = 02 + 02 + 02 + 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
488	$0250 + 03 = 02 + 02 + 02 + 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
489	$0250 + 62 = 02 + 02 + 02 + 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
490	$0250 + 80 = 02 + 02 + 02 + 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
491	$0250 + 125 = 02 + 02 + 02 + 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
492	$0250 + 02 = 02 + 02 + 02 + 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
493	$0250 + 02 = 02 + 02 + 02 + 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
494	$0250 + 03 = 02 + 02 + 02 + 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
495	$0250 + 04 = 02 + 02 + 02 + 02 + 02 + 02$	2.0E-07	-1.5	0	ESTIMATED
496		2.0E-07	-1.5	0	ESTIMATED

DATE OF LAST REACTION CHANGE IS JUNE 26, 1976

DATE OF LAST REFERENCE CHANGE IS JUNE 16, 1977

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